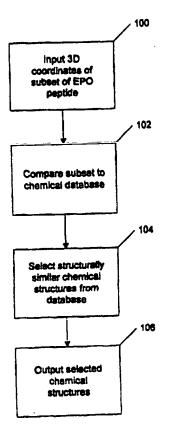


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(57) Abstract		100
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SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

BACKGROUND OF THE INVENTION

1. Field of the Invention

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This invention relates to computer-assisted methods for identifying and designing small molecule mimetics of erythropoietin.

2. Description of Related Art

Erythropoietin (EPO) is the primary regulator of the proliferation and differentiation of immature erythroid cells. EPO is produced in the fetal liver and in the adult kidney in response to hypoxia (low oxygen levels in blood or tissue). It circulates in the blood stream where it targets the EPO receptor (EPOR) on committed progenitor cells in the bone marrow and other hematopoietic tissues. Recombinant human erythropoietin (rHuEPO) is widely used in therapy of patients with anaemia due to chronic renal failure, cancer chemotherapy and AZT treatment.

The EPO receptor belongs to the cytokine receptor superfamily which includes receptors for other hematopoietic growth factors such as interleukins (ILs), colony stimulating factors (CSFs) as well as growth hormone prolactin and ciliary neurotrophic factor (CNTF). The structural architecture of this family of receptors consists of three modules: a ligand binding extracellular domain, a short trans membrane region and a large cytoplasmic domain. It has been proposed that the extracellular domain of this superfamily comprises two discrete domains each containing approximately 100 residues that fold into a sandwich consisting of 7 antiparallel β-strands with the topology of an Ig constant domain. Members of the family share two characteristic motifs in their extracellular domain: a pair of conserved disulfide bridges in the N-terminal domain, and a WSXWS box (where X is any amino acid residue) in the C-terminal domain. For most members of this receptor superfamily, oligomerization of one or more polypeptide chains

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is essential for forming high affinity receptor complexes. A homodimer complex has been demonstrated to be the active form of hGHR and a similar model has been suggested for G-CSF, prolactin and EPO receptors.

Erythropoietin induces dimerization of two EPO receptor molecules, which results in subsequent phosphorylation of the cytoplasmic domains by the association with two tyrosine kinase (JAK2) molecules to initiate a cascade of events that leads to the relevant biological.

Given the importance of erythropoietin, it would be very desirable to be able to identify molecules capable of binding the EPO receptor and eliciting the response normally elicited by EPO.

SUMMARY OF THE INVENTION

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The invention features methods for identifying molecules which will bind to the EPO receptor and act as a EPO mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity. Preferred mimetics are molecules lacking peptide bonds, i.e., are non peptidic mimetics. Preferred peptide mimetics have 15 or fewer, more preferably 10 or fewer amino acids.

The methods of the invention entail identification and design of molecules having a particular structure. The methods rely on the use of precise structural information derived from x-ray crystallographic studies of the extracellular domain of EPO receptor (amino acids 1 to 225) complexed with a peptide, EMP1 (EPO Mimetic Peptide 1; described below), which acts as an EPO mimetic. This crystallographic data permits the identification of atoms in the peptide mimetic that are important for EPO receptor binding and dimerization. More importantly, this data defines a three dimensional array of the important contact atoms. Other molecules which include a portion in which the atoms have a similar three dimensional arrangement similar to some or all of these contact atoms are likely to be capable of acting as an EPO mimetic. Moreover, one can use the structural information to design or identify molecules having even more EPO activity-than the peptide mimetic described herein.

The details of the preferred embodiment of the present invention are set forth in the accompanying drawings and the description below. Once the details of the invention are known, numerous additional innovations and changes will become obvious to one skilled in the art.

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BRIEF DESCRIPTION OF THE DRAWINGS

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FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system.

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system.

Like reference numbers and designations in the various drawings indicate like elements.

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DETAILED DESCRIPTION OF THE INVENTION

Throughout this description, the preferred embodiment and examples shown should be considered as exemplars, rather than as limitations on the present invention.

Described below is the crystal structure of a small peptide mimetic of EPO bound to an peptide, EMP1 **EPO** receptor. The of extracellular portion the (GGTYSCHFGPLTWVCKPQGG; SEQ ID NO:1), is characterized by an intramolecular disulfide bridge. Several lines of evidence suggest that EMP1 can act as an EPO mimetic. For example, EMP1 competes with EPO in receptor binding assays and induces cellular proliferation of cell lines engineered to be responsive to EPO. Both EPO and peptide induce a similar cascade of phosphorylation events and cell cycle progression in EPO responsive cells. Further, EMP1 demonstrates significant erythropoietic effects in mice as monitored by two different in vivo assays of nascent red blood cell production. This data, when combined, strongly supports the notion that the peptide ligand, which has a sequence unrelated to that of EPO, is capable of binding to and inducing an agonist conformation or assembly of EPO receptor.

Design of small molecule mimetics

The structure of the EMP1 dimer demonstrates that a molecule substantially smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide is assumed to have a substantially smaller contact interface with the receptor than its natural hormone. The binding determinants in the EPO receptor form an almost flat surface which is mainly hydrophobic in nature, without any cavities or charged residues that may help in design of a small molecule ligand to interact with the receptor.

This simplified framework of interactions revealed by the structural data presented herein can be used to identify additional EPO mimetics. The atoms of EMP1 which are important for binding to the EPO receptor and forming dimeric EPO receptor include those involved in the contact between the EMP1 (peptide) and EBP (EPO receptor) and

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those involved in contacts between the two EMP1 molecules in the dimeric complex (peptide-peptide contacts). In addition to the contacts listed in Table 2, the following EMP1-EMP1 hydrophobic contacts are significant: Tyr^{P4}, Cys^{P6}, Phe^{P8}, Trp^{P13}, and Cys^{P13} in each peptide. The following EMP1-EBP hydrophobic interactions are also significant: Tyr^{P4}, Phe^{P8}, and Trp^{P13} in each peptide. It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a mimetic. In fact, it is only those few atoms which actually from important contacts with the EPO receptor which are likely to be important for mimetic activity. Those skilled in the art will be able to identify these important atoms based on the model of the dimeric EMP1-EPO complex which can be constructed using the structural data herein.

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Preferred mimetics will include atoms at postions similar to those of the EPO receptor contacting atoms of EMP1. Even more preferred mimetics will be structurally similar to the dimer of EMP1 found in the structure described below. This is because the dimerization of EMP1 is an important factor in the diemerization of the EPO receptor.

The methods of the invention employ a computer-based methods for identifying 15 compounds having a desired structure. More specifically, the invention uses the threedimensional coordinates of a subset of the atoms in the GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the human EPO receptor, to determine peptide and non-peptide mimetic candidates by means of computer methods. 20

These computer-based methods fall into two broad classes: database methods and *de novo* design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional (*i.e.*, sequence)

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data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g., data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atom-by-atom manner or by assembling stored small molecular fragments.

The success of both database and de novo methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally relevant portion of the compound of interest. For drugs, the functionally relevant portion is referred to a pharmacophore. A pharmacophore then is an arrangement of structural features and functional groups important for biological activity, e.g., EPO activity.

Not all identified compounds having the desired pharmacophore will act as an EPO mimetic. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds which must be tested to identify an actual mimetic.

Dimerization of the EPO receptor is important for activity. Accordingly, preferred mimetics will be based on the structure of the EMP1 dimer as it is bound to the EPO receptor dimer. Thus, preferred mimetics have include important contacts from both of the RWJ 61233 peptides present in the structure described below. Such mimetics will favor dimerization of the EPO receptor.

Programs suitable for generating predicted three-dimensional structures from two-dimensional data include: Concord (Tripos Associated, St. Louis, MO), 3-D Builder (Chemical Design Ltd., Oxford, U.K.), Catalyst (Bio-CAD Corp., Mountain View, CA), and Daylight (Abbott Laboratories, Abbott Park, IL).

Programs suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore include: MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB Unity (Tripos Associates, St. Louis, MO).

Programs suitable for pharmacophore selection and design include: DISCO (Abbott Laboratories, Abbott Park, IL), Catalyst (Bio-CAD Corp., Mountain View, CA), and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

Databases of chemical structures are available from Cambridge Crystallographic Data Centre (Cambridge, U.K.) and Chemical Abstracts Service (Columbus, OH).

De novo design programs include Ludi (Biosym Technologies Inc., San Diego, CA) and Aladdin (Daylight Chemical Information Systems, Irvine CA).

Those skilled in the art will recognize that the design of a mimetic may require slight structural alteration or adjustment of a chemical structure designed or identified using the methods of the invention.

- In general, chemical compounds identified or designed using the methods of the invention can be sythesized chemically and then tested for EPO activity using any of the methods described below. The methods of the invention are particularly useful because they can be used to greatly decrease the number potential mimetics which must be screened for EPO activity.
- The invention may be implemented in hardware or software, or a combination of both. However, preferably, the invention is implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions

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described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The inventive system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 100);
- comparing, using the processor, the criteria data set to a computer database of chemical structures stored in the computer data storage system (STEP 102);

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- (3) selecting from the database, using a program suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore (such as those described above or equivalents), chemical structures having a portion that is structurally similar to the criteria data set (STEP 104);
- outputting to an output device the selected chemical structures having a portion similar to the criteria data set (STEP 106).

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 200);
- (2) constructing, using a program suitable for generating chemical structure models (such as those described above or equivalents), a model of a chemical structure having a portion that is structurally similar to the criteria data set (STEP 202);
- (3) outputting to the output device the constructed model (STEP 204).

20 Confirmation of Biological Activity

In order to determine whether a molecule identified using the methods of the invention can act as an EPO mimetic, one or more *in vitro* or *in vivo* assays of EPO activity should be performed. For example, mimetic molecules should be able to stimulate proliferation of TF-1 cells (Kitamura et al., J. Cell Physiol. 140:323, 1985) or B6Sut cells (Greenberger et al., Proc. Natl. Acad. Sci. USA 80:2931, 1983), but preferably do not stimulate proliferation of cells which do not bear the EPO receptor. Thus, preferred mimetics do not stimulate proliferation of Mo7e cells (Avanzi et al., Br. J. Haematol. 69:359, 1988).

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Potential mimetics can also be tested in a murine model of erythropoiesis. In this assay a potential mimetic is administered to normal mice which express endogenous basal levels of EPO. Reticulocytes are counted, preferably by flow cytometry, to determine whether the candidate mimetic increases reticulocyte levels. An increase in reticulocyte levels indicates that the candidate mimetic is stimulating erythropoiesis. Because the mice used in this assay already express EPO, this assay may be relatively insensitive. As an alternative, candidate mimetics can be assayed in the exhypoxic-polycythemic mouse bioassay. In this assay polycythemia is induced by conditioning mice in a hypobaric chamber to reduce endogenous EPO levels. A potential EPO mimetic can be administered to a conditioned mouse. Incorporation of ⁵⁹Fe into blood serves as a measure of erythropoiesis. This erythropoiesis can be attributed to the candidate mimetic.

The assays described above are examples of suitable assays. Other assays for EPO activity known to those skilled in the art are also useful.

In order to determine the biological activity of a candidate mimetic it is preferable to measure biological activity at several concentrations of candidate mimetic. The activity at a given concentration of candidate mimetic can be compared to the activity of EPO itself.

Structural Data

The coordinates for amino acids 1 to 225 of the human EPO receptor bound to peptide EMP1 are presented in the attached appendix in standard Brookhaven database format. Also included in this appendix is a list of van der Waals interactions. These coordinates can be used in the design and identification of EPO mimetics according to the methods of the invention.

Structure of EBP-EMP1 Complex

The extracellular fragment of human EPO receptor (EPO binding protein, EBP), consisting of residues 1-225, was expressed in Escherichia coli and purified as described

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(Johnson et al., Protein Express. Purif. 7:104, 1996). Rhomboidal-shaped crystals of an EBP complex with EMP1 were obtained in orthorhombic space group P2₁2₁2₁, with cell parameters a=59.2Å, b=75.5Å, c=132.2Å, with two EBP and two peptide molecules in the asymmetric unit and a V_N=2.8 Å'/dalton (Matthews, J. Mol. Biol. 33:491, 1968). The crystal structure was determined by multiple isomorphous replacement (MIR) using two heavy atom derivatives (Table 1). Residues 1-2 and 19-20 of each peptide as well as residues 1-9, 21-23, 164-166, 221-225 of receptor molecule I, and residues 1-9, 21-23, 133-135, 221-225 of receptor molecule II had poor or no electron density and are excluded from the structure analyses

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An important break in the electron density that affects the structure interpretation occurs for the three residues (Arg¹¹ -Gly²² -Pro²³) that link the amino terminal α -helix to the first β-strand in D1 of both receptor molecules. A molecular packing diagram shows the proximity of a second non-crystallographically related dimer in the crystal that gives two possibilities of how this three-residue linker may be connected. The current choice of linker connectivity is based on a structure of another independent EBP-peptide complex at higher resolution (2.5 Å), which shares a similar molecular packing, but for which the electron density is clear for these three residues. At present there are no experimental data to verify whether this N-terminal \alpha-helix exists in solution or is a crystallization packing artifact. Notably, this helical region is not observed in the published structures of hGHbp (begins at residue 32; deVos et al., Science 255:306, 1992), PRLR (begins at residue 2, without any defined secondary structure until the first β -strand, residue 6; Somers et al., Nature 372:478, 1994), the INF-yRa (begins at residue 17; Walter et al., Nature 376:230, 1995) or the tissue factor (begins at residue 3 without any defined secondary structure until the first β-strand, residue 11; Muller et al., Nature 370:662, 1994).

The EBP monomer folds into two domains, D1 and D2, that form an L-shape with the long axis of each domain aligned at approximately 90° to each other; the overall molecular dimensions are 45 Å x 52 Å x 62 Å. The N-terminal domain (D1, residues 10-

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114) and C-terminal domain (D2, residues 119-220) are connected by a short four residue α-helix linker. Both domains are more closely related in overall topology to Fibronectin type-III (FBN-III) domains than to Ig domains (Bork et al., J. Mol. Biol., 242:309, 1994). The FBN-III fold is composed of two antiparallel β -pleated sheets, consisting of strands A, B, E and strands G, F, C and C', and is found in the two domains of the human growth hormone (de Vos et al., Science 255:306, 1992) and prolactin (Somers et al., Nature 372:478, 1994) receptors, the D1 and D2 domains of the α chain of interferon- γ receptor (IFN-YRa) (Walter et al., Nature 376:230, 1995), the D2 domain of CD4 (Wang et al, Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the two domains of tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), the third fibronectin-type repeat of tenacin (Leagy et al., Science 258:987, 1992) and the D2 domain of the chaperone protein PapD (Holmgren et al., Nature 342:248, 1989). The FBN-III topology differs from an Ig constant domain by a shift of strand D from one βsheet (strands A, B, E and D) to the other (strands G, F, C, C'), where it is defined as the C' strand. Superposition of equivalent β -sheet core residues of the D1 and D2 domains in EBP gives an r.m.s. deviation of 2.3 Å for 77 Ca pairs, which is significantly larger than the corresponding domain overlaps for hGHbp (1.1Å) and PRLR (0.8Å), and reflects a difference in the subclass of fold between the two EBP domains.

In D1, a short α -helix (residues 10-20), precedes the first β -sandwich that is better described as a hybrid of the FBN-III fold with an Ig fold (residues 24-114), rather than strict FBN-III topology. In this h-type fold (Wang et al., Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the C' strand is long and interacts first with strand C and then switches to interact with strand E (where C' changes its designation to strand D) forming a four-on-four strand β -sandwich. D1 contains the two conserved disulfide bridges linking Cys 11 (β A) to Cys 11 (β B) and Cys 11 (β C') to Cys 11 (β E). The number of residues between the cysteine pairs that form the two disulfide bridges are 9 and 15 for EBP, compared to 9 and 10 in both GHR and PRLR. The longer connection between strands C' and E enables the second half of strand C' to become strand D. This h-type topology is not found in either of the two s-type GHR domains. A potential glycoylation site exists

on residue Asn^{52} which is located towards the end of the loop region connecting the βB and βC strands. Although Asn^{52} is not glycosylated in this bacterially expressed protein, an external cavity around the Asn^{52} side chain could easily accommodate a carbohydrate moiety.

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A helical linker (residues 115-118) connects D1 to D2 (The φ, Ψ torsion angles for the interdomain helical linker for lle¹¹³, Asn¹¹⁴, Glu¹¹⁷ and Val¹⁴ are -50° -27°, -76°, -21°, -99°, 26°, and -151°, 38° respectively.) and has been observed in other members of this receptor family, hGHbp, PRLR, IFN-γRα and tissue factor. In EBP, the domain association is further restricted by a mixed assortment of hydrogen bonding, hydrophobic interactions and one salt bridge (between Arg¹² and Asp¹²) from 11 residues of D1 and 12 residues of D2 with a total buried surface [The molecular surface areas buried by interaction were calculated using the program MS (Connolly, J. Appl. Crystallog, 16:439, 1983) using a 1.7Å probe sphere and standard atomic radii (as described in Davies, et al, Ann. Rev. Biochem. 59:439, 1990). There may be some discrepancies between values reported here and other (deVos et al., Scince 255:306, 1992) published values due to use of a different algorithm (Connolly) vs. Lee et al., J. Mol. Biol., 55: 379, 1971) and probe radii. For clarity all values reported here have been calculated in the same way for better comparison between the receptors] of 950 Å² for the two domains.

D2 (residues 119-220) folds into the standard FBN-III (s-type) topology with one free cysteine and no disulfide bridges, consistent with GHR and PRLR that have three and two disulfide bridges, respectively, in D1 but none in D2. After the α -helix linker, D2 begins with an irregular coil (residues 118-126) that contains Pro^{124} which is conserved in the structures of hGHbp, PRLR, tissue factor and IFN γ -R α , and based on sequence alignment, in most class-1 and class-2 cytokine receptors (Bazan, Proc. Natl. Acad. Sci. USA 87:6934, 1990). This short coil ends with Gly¹²⁴ which has a positive ϕ (ϕ , $\Psi \approx 52^{\circ}$,40°) consistent with the equivalent Ala¹³⁶ and Ala¹⁰¹ torsion angles in hGHbp (ϕ , $\Psi \approx 63^{\circ}$,68°) and PRLR (ϕ , $\Psi \approx 58^{\circ}$,38°). The Pro¹²⁴ region forms an analogous extended bulge conformation adjacent and parallel to a corresponding bulge containing the

WSXWS motif. The WSAWS sequence forms a modified wide β -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981) and is located in an extended chain region immediately preceding the βG strand that would normally connect to the membrane spanning region of the EPOR.

The quaternary structure of the complex is composed of two peptides and two receptors that form a T-shapes assembly. A noncovalent peptide dimer interacts with two receptor molecules to generate an almost perfect 2-fold symmetrical arrangement. After superposition of D2 of the two EBP molecules in the dimer, the centers of mass of the two D1 domains are only 0.8 Å apart, sufficient to perturb perfect two-fold symmetry. Separate superposition of the corresponding D1 and D2 of each receptor in the dimer results in r.m.s. deviations of 0.53 Å (105 D1 Ca pairs) and 0.47 Å (93 D2 Ca pairs).

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The cyclic EMP1 contains a single disulfide bridge between Cys^{P6} and Cys^{P15}, which links two short β-strands (residues 4-7 and 13-16) that are connected by a slightly distorted type 1 β -turn [Pro^{P10} (i+1) and Leu^{P11} (i+2) of the β -turn have $\dot{\phi}, \Psi \approx -62^{\circ}$, -38° and -99°, -60° respectively. The carbonyl oxygen of LeuP11 has a hydrogen bond to EBP distorting the Ψ value from its normal 0°±30° (i+2) in a standard type I β-turn.] consisting of residues Gly^{P9}-Pro^{P10}-Leu^{P11}-Thr^{P12}. Each peptide has a very close association with its other peptide partner and buries 320 Å of its 1220 Å² molecular surface in this interaction (Connelly, J. Appl. Crystallog. 16:439, 1983; Davies et al., Ann. Rev. Biochem. 59:439, 1990; Richards, J. Mol. Biol. 55:379, 1971). Four hydrogen bonds between the mainchains of the two peptides results in formation of a four-stranded anti-parallel βpleated sheet (Table 2). Two symmetric hyrdophobic cores are assembled by peptide dimerization and are comprised of the disulfide bridges and the side chains of Tyr^{P4}, Phe^{P2} and Trp^{P13}. The construction of each hydrophobic core resembles a box which places the aromatic rings of PheP4, TrpP13 and TyrP4 (from the other peptide) and the disulfide bridge (Cys^{P6}-Cys^{P15}) at the corners. The two glycine residues at either end of the peptide are not structured.

The peptide dimer is embedded in a deep crevice between two EBP receptor molecules. A portion of each peptide monomer interacts with both receptor molecules. The binding sites of each EBP are practically identical due to the 2-fold symmetric interactions imposed on binding the peptide dimer. The four major contact areas on EBP come from segments on four loop regions (L1, L3, L5, L6) that connect strands A to B (L1 residues 33-34) and F to G (L6 residues 90-94) in D1 and strands B to C (L5 residues 148-153) and F to G (L6 residues 203-205) in D2. The total buried molecular surfaces in the peptide-EBP assembly are 840 Å² and 880 Å² for the two peptides and EBP's, respectively. The peptide-EBP interaction can be separated into distinct hydrophobic (67%) and polar (33%) areas. A hydrophobic core is formed between the peptide and receptor and comprises Phe93, Met150 and Phe205 from one EBP molecule and the peptide hydrophobic box consisting of PheP8 and TrpP13 from one peptide and TyrP4 and CysP15 from the other peptide. The polar interactions are located mainly at the bottom of the binding crevice and are mainly with loop L5 in D2. Five of the six hydrogen bonds are between the mainchain of the β-turn residues Gly^{P9}, Pro^{P10} and Leg^{P11} from one peptide with the mainchain and sidechain hydroxyl of conserved TyrP4, which crosses over its other peptide partner, to interact with loop L3 (Table 2). The EBP-EBP interaction makes a surprisingly minor contribution to the overall stability of the complex where the interreceptor buried molecular surface is only 75 Å², contributed by Leu¹⁷⁵ and Arg¹⁷⁸ from each receptor molecule.

EMP1 is one of a family of sequences that contain several conserved residues, besides the cysteines (ELANGE, PERSONAL TESSES, PESS). The most structurally significant of these consensus residues appear to be Tyr^{P4} and Trp^{P13}, which along with the disulfide bridge have a major contribution to the hydrophobic core of the peptide-peptide interaction. Moreover, these two aromatic residues play a pivotal role in peptide-receptor interaction and in receptor dimerization.

Dimerization of EBP in Solution

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To explore the interaction of EMP1 with EBP in solution we employed a [1,4-di-(2'-pyridyldithio DPDPB. bifunctionalsulphydryl reactive crosslinker propionamido) butane], in an attempt to stabilize a peptide-dependent dimeric structure. The choice of crosslinker was based on previous experiments with amine-reactive crosslinkers that were found to inactivate EBP. EBP contains a single free sulphydryl (Cys¹⁸¹) in D2 which is potentially reactive to crosslinking reagents (The DPDPB crosslinker itself does not inactivate the EPO binding potential of EBP nor the proliferative properties of EMP1). A dimeric EBP product is formed by co-incubation of EMP1, DPDPB and EBP. The amount of dimeric product increases with peptide concentration and no significant dimer product is observed in the absence of peptide. DPDPB-crosslinked products formed through disulfide-exchange reactions should be readily reversible by reduction as is seen for the covalently-linked EMP1-mediated dimer. Furthermore, we have constructed a covalently-linked dimeric form of EMP1 that demonstrates increased biological potency (Johnson et al, in preparation). The Cys¹⁸¹ residues in D2 of the EBP dimer are 20.7 Å apart (Sy-Sy distance) which approximates the 16 Å length (and approximately 2 Å in bond length at each end) of the DPDPB crosslinker. Thus EMP1 mediates formation of a soluble EBP dimer complex in solution consistent with the crystal structure.

The WSXWS motif

The WSAWS sequence (residues 209-213) corresponding to the WSXWS box occurs in a β -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) immediately preceding β -strand G in D2. Residues in this motif do not interact with ligand, have no role in receptor-receptor interactions and are located on the opposite side of the receptor-receptor and receptor-ligand interface. The WSAWS box represents only a segment of a complex array of interactions that involves several other conserved side chains from the four-stranded β -sheet in D2. The indole ring systems of Trp²⁰⁹ and Trp²¹² point toward an external concave surface of the β -sheet and are only partially solvent exposed, whereas the Ala²¹¹ side chain points directly out into solution. The amides and hydroxyls of both Ser²¹⁰ and Ser²¹³ form hydrogen bonds with the main

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chain of residues 198 and 196 of adjacent strand F in a pseudo β -sheet type interaction that resembles a modified wide β-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) where the sidechain hydroxyl rather than the carbonyl oxygen makes the β -sheet interaction. The β -bulge architecture places the two Trp residues, which are spread four residues apart, on the same side of the β -sheet and not on opposite sides as in normal β-sheet or extended chain structures. The guanidinum group of Arg¹⁹⁷ from Strand F, the central residue (Richardson, Adv. Prot. Chem. 34: 167, 1981; Chan et al., Protein Science, 2:1574, 1993) in the bulge, is positioned exactly between the two Trp indole rings to form an extended π -cation system (Kumpf et al., Science 261:1708, 1993. The center of the pyrrole ring of Trp²⁰⁹, the NE of the Arg¹⁹⁷ and the center of the benzene ring of Trp212 are positioned on a straight line with the three planes of the conjugated systems stacked parallel to each other at approximately 4 Å spacing. In addition, the aliphatic portion of the Arg¹⁹⁹ side chain has hydrophobic interactions with the indole ring of Trp²⁰⁹, completing the alternating stacking of two aromatic and two positively-charged amino acid residues. The side chain of Glu¹⁵⁷ forms a hydrogen bond with Arg¹⁹⁷ presumably to help orient the guanidinium group and add some specificity and stabilization to the system.

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It appears then that the linear WSXWS motif identified from sequence alignments of cytokine receptors represents only a component of a more complex conformational unit that contributes a significant structural feature to D2. Aromatic residues have previously been suggested to have a stabilizing effect and play a role as a folding nuclei in structures of antiparallel β -sandwiches (Finkelstein et al., Protein Eng. 6:367, 1993). The aminoaromatic parallel stacking between the guanidinium group of arginine and the aromatic rings is a common feature in protein structures (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994), but a parallel triple stacking of π -cation systems is rare (Kim et al., Biochemistry 32:8465, 1993) although observed in other class-1 cytokine receptors, hGHbp and PRLR.

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The structural equivalents of the WSXWS motif in hGHbp (YGEFS) and PRLR (WSAWS) are involved in an even more intricate and complex array of π -cation interactions. The π -cation system is extended in hGHbp and PRLR to include an additional aromatic residue (Trp186 for hGHbp and Trp186 for PRLR) from the loop region that links βC and $\beta C'$ in D2 and a positively-charged residue (Arg²¹¹ for hGHbp and Arg147 for PRLR) that stacks between the Trp and the second aromatic residue. The additional Arg residue is contributed either from the βF strand as in hGHbp (Arg²¹¹) or from βC as in PRLR (Arg¹⁴⁷); the glutamine residue that hydrogen bonds and orients the arginine also switches strands. Sequence alignments suggest that this Arg-Gln switch could be common to other members of the class-1 cytokine receptor family. The extended π -cation system in hGHbp and PRLR consists of five positively charged and three aromatic residues stacked in an alternating order which comprises of Lys215, Tyr222, Arg²¹³, Phe²²⁵, Arg²¹¹, Trp¹⁸⁶, Lys¹⁷⁹ for hGHbp and Lys¹⁸⁵, Trp¹⁹¹, Arg¹⁸³, Trp¹⁹⁴, Arg¹⁴⁷, Trp156, Lys149 for PRLR. The first aromatic-Arg-aromatic trio are approximately 4Å apart, as in EBP, but the second system is stacked closer together at approximately 3.6 Å spacings consistent with π - π interaction (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994). The outer lysines also use the aliphatic portions of their side chains to form hydrophobic interactions with the aromatic rings. Based on sequence alignments with other members of the class-1 cytokine receptor superfamily, such structurally extended π -cation systems could exist in human thrombopietin, IL-6 and ciliary neurotrophic factor receptors, and in human IL-4 receptor based on structural modeling (Gustchina et al., Proteins 21:140, 1995). Although IFNγRα and tissue factor do not have a WSXWS motif, the corresponding sequences TTEKS (residues 213-217) for IFN-YRa (Walter et al., Nature 376:230, 1995) and KSTDS (residues 201-205) for tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), maintain a very similar β -bulge. The consensus sequence among these five x-ray structures indicates that a serine or threonine in positions 2 and 5 maintain a common set of hydrogen bonds between their side chain hydroxyls and the mainchain of the neighboring strand. Only in hGHbp is there no hydroxyl-containing residue in position 2, but Ser²²⁶ still maintains the equivalent interaction. A Ser²²⁶ to Ala

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mutation abrogates hGHR binding to hGH, and its expression on the cell surface is drastically reduced (Baumgartner et al., J. Biol. Chem., 269: 29094, 1994). In GM-CSFR α and IL-2R β , point mutations of the serine residues cause a substantial decrease in cell surface expression but little or no effect on ligand binding (Ronco et al., J. Biol. Chem. 269:277, 1994; Miyazaki et al., EMBO Journal 10:3191, 1991).

Conservation of the WSXWS motif in EPOR or its equivalent in other members of the class 1 cytokine receptors has been proposed to be essential for biological activity and was thus assumed to be part of the receptor binding site (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle, Mol. Cell. Biol. 12:4553 1992). For EPOR, a systematic study of 100 mutations of the WSAWS sequence demonstrates that most of the mutations of the two tryptophan and serine resulted in molecules that did not reach the cell surface but were retained in the endoplasmatic reticulum (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). Furthermore, an Ala²¹¹ to Glu mutation in the WSAWS sequence resulted in better transportation from the ER to the Golgi and a 3-5 fold increase of the number of EPOR molecules on the cell surface compared to the wild-type (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). These results support our conclusion that the WSXWS sequence plays an important role in the structure and folding of D2 in EPOR and other related receptors.

20 Comparison with other cytokine-receptor complex structures

The overall quaternary structure of the peptide-EBP complex substantially from the equivalent arrangement in the hGH-hGHR complex. The non-symmetric nature of the single four-helix-bundle structure of the growth hormone ligand results in an asymmetric homo-dimerization of the receptor that corresponds to a 159° rotation between receptors compared to the almost perfect 2-fold (180°) rotation for the EBP-peptide complex. The tertiary arrangement of domains within EBP and hGHbp is also somewhat different. When the equivalent EBP and hGHbp D2 domains are superimposed on each other, their corresponding D1 domains differ by a 12° rotation and a 4.3Å translation.

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The mechanism of hGH binding to its receptor has been well studied (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) and is sequential. Initial high affinity (nM) binding of the hormone with one receptor results is a buried surface of 1130 ${\rm Å}^2$ on the receptor. The second hGHbp2 has a substantially smaller interface (deVos et al., Science 255:306, 1992) with the second binding site on hGH and interacts only with the preformed 1:1 complex to generate buried surface areas of 740 ${\rm Å}^2$ with hGH and 440 ${\rm Å}^2$ with the first hGHbp1 (deVos et al., Science 255:306, 1992; (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995). The binding determinants of each hGHbp are comprised of the six recognition loops (L1-L6), three of which (L1-L3) come from one end of the ${\rm \beta}$ -sandwich structure in D1, one from the interdomain linker and two from D2.

Although these two receptor complexes, EBP-EMP1 and hGH-hGHbp, have different dimeric arrangements, which probably in this case represent differences in the size and shape of the natural versus synthetic ligand, both receptors share equivalent ligand recognition loops, L1, L3, L5 and L6 for the EBP and L1 to L6 for the hGHbp. A nonactive PRLR, complexed with only one molecule of hGH, also uses the same contact loops (L1 to L6) (Somers et al., Nature 372:478, 1994). Based on similarity of the ligand recognition sites in hGHbp and PRLR, one would expect that the binding site of EBP, when its natural EPO ligand is bound, would extend to include two additional loops, L2 and L4, that comprise residues 59-63 (L2) between strands C to C', and residues 110-118 (L4) from the carboxyl end of βG in D1 and the interdomain linker. These six loops in EBP, hGHbp and PRLR area in structurally equivalent positions but vary in size, amino acid composition and conformation although the interacting portions of each loop (side or tip) remain similar; L1, L2, L3, L5 interact mainly with their tips and L6 with its side. In EBP, the L5 loop is three residues shorter than in hGHbp and PRLR, where the L6 loop is three and four residues longer than in hGHbp and PRLR, respectively. The L2 loop also varies (6 to 10 residues) among the three receptors but in EBP does not participate in peptide binding, and in hGHbp is partially disordered, although it does contact the hormone. In one respect, this situation is similar to the complementaritydetermining regions (CDR's) in antibodies, where changes in length and sequence of the six binding loops impose specificity for different antigens, whereas the framework itself remains constant (Wilson et al., Ciba Foundation Symposium. Wiley, Chichester, 1991, Vol. 159, p. 13).

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It has been shown for the hGH-hGHbp complex that only a subset of 9 out of 33 interacting residues that make up the structural epitope of the receptor constitute a functional epitope or hot spot (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) where high affinity binding interaction takes place. This reduced epitope is substantially smaller than the structural epitope and is comprised from residues (Arg43, Glu44, Ile103, Trp104, Ile105, Pro106, Asp165, and Trp169) which are located in contact loops L1, L3 and L5 with the most significant contribution (>4.5 kcal/mol) coming from two aromatic residues (Trp104 and Trp169) in L3 and L5 (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996). In EBP, Phe⁹³ is equivalent to Trp¹⁰⁴ in hGHbp, as suggested previously (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996; Jolliffe et al., Nephrol. Dial. Trans. 10; suppl. 2, 28, 1995), but there is no homologous residue to Trp¹⁶⁹ in the shorter L5 loop. In the EBP-EMP1 complex, the PhePt peptide aromatic side chain occupies the equivalent position of the Trp 169 side chain in hGHbp. One can assume that when EPO binds to its receptor, the hormone may provide an aromatic residue to the hydrophobic core of the binding interface and/or the L6 loop in EBP may play a more significant role in the hormone binding than in hGHbp, since it is 3 residues longer and contains the aromatic Phe²⁰⁵.

In these three class-1 receptor structures, some loops are disordered which are in D2 for EBP for EBP (residues 164-166 in EBP1 and 133-135 in EBP2) and in D1 for both hGHbp (residues 55-58, 73-78 for hGHbp1 and 54-60, 73-75 for hGHbp2) and PRLR (residues 31-33, 84-86). Otherwise, these three class-1 cytokine receptors do not differ greatly in their over all tertiary structures; D1 and D2 have broadly similar general

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arrangement in all three receptors such that the angle between the long axes of the two domains is approximately 90 degrees. I tis this arrangement of domains that allow these particular L1-L6 loops to be available for the recognition and binding of ligands. In a 2:2 complex between IFN-γ and its class-2 receptor IFN-γRα, D1 and D2 are related by a 125 degree angle, which elongates the receptor and restricts the binding determinants that can be used for interaction with hormone; the L1 loop now becomes buried in the D1-D2 interface, although the other five loops (L2-L6) are still available for ligand interaction. This elongated interdomain arrangement is also observed in tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994) which has a distant relationship to the cytokine receptor superfamily.

A mutational analysis of the EBP molecule indicates that the most crucial amino acid residue for binding EPO is Phe⁹³ in the L3 loop (Jolliffe et al., Nephrol. Dial. Trans. 10:suppl 2,28, 1995). The Phe93Ala mutant shows an increase int he IC₅₀ compared to the wild-type by a factor of approximately 1000, whereas other mutants (Ser91Ala, Ser92Ala, Val94Ala, Met150Ala and His153Ala) show small relative increases in teh IC₅₀ of only 2.5-12.5 fold). The side chain of Phe⁹³ buries 66 Å² of molecular surface, which is the highest among interacting side chains. In hGHbp, the corresponding Trp104Ala mutation results in an increase in the K_d by a factor of more than 2,500 compared to the wild-type indicating the equivalent importance of this residue in hGH binding and its key contribution to the hydrophobic core of the functional epitope (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Bass et al. Proc. Natl. Acad. Sci. USA 88:4498, 1991).

The role of dimerization on signal transduction

In the EBP-EMP1 complex structure, we surprisingly observe that a peptide, unrelated in sequence and probably in structure, to the natural ligand, can induce a biologically active dimerization of EPO receptor that promotes signal transduction and cell proliferation. Comparison of three class-1 cytokine receptor complexes, whose structures have been determined so far, suggests that when the natural EPO hormone, which is

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proposed to have a structure of a four-helix bundle (Boissel et al., J. Biol. Chem. 268:15983, 1993), induces receptor dimerization, it is more likely to resemble the hGH-hGHbp assemblage. This would suggest that more than one mode of productive extracellular dimerization is permissive for intracellular dimerization of the cytoplasmic domains with two JAK2 molecules in order to initialize the cascade of events that produces the biologically relevant signal (Ihle et al., Seminars in Immunology 5:375, 1993; Klingmuller et al., Cell 80:729, 1995). The peptide-EBP structure would then represent only one possible dimeric arrangement that promotes signal transduction.

Mutant EPOR molecules, containing a single Arg to Cys mutation (Arg¹³⁰ in human and Arg¹²⁹ in murine), have been shown to form biologically active dimers in the absence of EPO (Yoshimura et al., J. Biol. Chem. 267:11619, 1992); Watowich et al., Proc. Natl. Acad. Sci. USA 89:2140, 1992; Watowich et al., Mol. Cell. Biol. 14:3535, 1994), suggesting that extracellular recptor homo-dimerization may be sufficient in itself for signal transduction. It has been shown in another system (Spencer et al., Science 262:1019, 1993) that activation of a specific set of transcription factors can be induced by the chemical crosslinking of cytoplasmic domains of modified cell membrane receptors that do not contain the extracellular and transmembrane domains. These receptors are not related to the cytokine receptor superfamily but illustrate that oligomerication plays a key role in activation of the receptor, and that the main functional role of the extracellular, ligand-binding domain is to allow (in the presence of ligand) dimerization or oligomerization and induce similar association of the cytoplasmic domains.

Mutageneses experiments originally suggested a role for the WSXWS motif in this cell signalling process (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle et al. Mol. Cell. Biol. 12:4553, 1992; Chiba et al., Biochem. Biophys. Res. Comm. 184:485, 1992) possibly by promoting receptor homo-dimerization. However, truncation mutants of EPOR (Miura et al., Arch. Biochem. Biophys. 306:200, 1993) do not confirm this role for the WSXWS motif. The EBP-EMP1 complex structure shows that the WSXWS motif

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of the EPOR, as for the hGH-hGHbp complex (deVos et al., Science 255:306, 1992) is located on the opposite face of the molecule from the receptor dimerization. In the absence of unliganded structures for the extracellular domains of EPOR, hGHR and PRLR, it is not possible to determine whether any conformation change occurs on ligand binding that would involve the WSXWS box. Apart from being a striking structural feature in D2, and its obvious proximity to the membrane spanning domain, one cannot rule out possible interactions of this region with some other cell surface molecules that are involved somehow in the signal transduction process.

Towards design of small molecule mimetics

The structure of the EMP1 dimer demonstrates that a peptide considerably smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide can be assumed to form a substantially smaller contact interface than the natural hormone with the receptor. The peptide binding site in EBP forms an almost flat surface, which is mainly hydrophobic in nature, without any cavities or charged residues that are normally essential for the specific targeting of small molecule ligands to a receptor binding site. The hGHbp study (Wells et al., Science 267:383, 1995; Wells, Proc. Natl. Acad. Sci. USA 93:1, 1996) shows that only a small part of the observed structural binding site, the so-called functional epitope (supra), contributes most of the binding energy and strongly implied that a "minimized" hormone designed to interact with this site could form sufficient interactions to activate the receptor. Furthermore, the limited site of interaction of the small agonist peptide with the EBP corresponds almost exactly to the smaller functional epitope derived from alarine scanning of hGH and hGHbp. Thus, by a different approach, we have arrived at the similar conclusion that a small number of key interactions can contribute to a functional epitope on a receptor. Understanding of this simplified interaction surface can be now combined with further mutational studies to assist in identifying the most crucial residues in the functional epitope, and consequently provide a more practical target for drug design.

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The crystallographic data is summarized in Table 1. Native crystallographic data were collected on a Siemens multiwire area detector mounted on an Elliott GX-18 generator, operating at 40kV and 55mA, with a crystal-to-detector distance of 120mm. Two derivative data sets were collected on a MAR image plate mounted on a Siemens generator operating at 50kV and 80mA, with crystal-to-image plate distance of 150mm. Data were integrated, scaled and reduced using the programs XENGEN (Howard et al., J. App. Cryst. 20:383, 1987) for the native data and DENZO/SCALEPACK (Otwinowski et al., SERC Darsbury Laboratory, Warrington, 1993) for the derivative data. Initial multiple isomorphous replacement anomalous scattering (MIRAS) phases were calculated to 3.1 Å using the program package PHASES (Furey, American Crystallographic Association Fortieth Anniversary Meeting, New Orleans, LA, 1990) with a mean figure of merit of 0.64 (25.0-3.1 Å). Phases were refined in PHASES using the solvent flattening protocol to a mean figure of merit of 0.92 (25.0-3.1 Å). The quality of the map was generally good and most of the complex structure (94%) could be fitted using the graphics program O (Jone et al., Acta Crystallogr A47:110, 1991). The register of the amino acid residues was verified from the positions of the two disulfide bridges in D1. and the positions of the two Hg's from the mercury acetate derivative that were correctly assumed to bind to the free Cys¹⁸¹ residue. the peptide interpretation was verified from another data set from a complex between EBP and an iodinated peptide (TyrP4 was substituted for p-iodo-Phe), which diffracted to 3.3Å resolution, that in difference Fourier (Find-Fm) and gave a clear indication of the location of the iodine atoms. The structure was refined using the slow-cooling protocol in X-PLOR 3.1(Brunger et al., Acta Crystallogr A46:585, 1990; Brunger, X-PLOR, Version 3.1: A System for X-ray and NMR, Yale Univ. Press, New Haven, CT, 1992) and rebuilt using Fo-Fc, 3Fo-2Fc and SIGMAA(Read, Acta Crystallogr. A42:140, 1986) weighted electron density maps. After every two cycles of refinement, a set of simulated annealing omit maps (7-10%) to reduce model bias was calculated and the entire structure rebuilt. After several cycles of refinement, individual temperature factors were calculated and after 10 cycles of refinement and model building, the R-value was 0.21 for 8.0-2.8 Å data with F>10 (13,984 reflections). The average thermal parameters for receptor I, receptor II and the

peptides are 10.5Å², 12.3Å and 10.7Å respectively. Only one non-glycine residue [Asn¹⁶⁴ in EBP2], located in a loop region in D1, is in a disallowed region in the Ramachandran plot. No solvent molecules were included in the model due to the moderate resolution (2.8 Å) of the structure determination.

5 Binding Contacts

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Binding contacts are summarized, in part, in Table 2: Hydrogen bond interactions in the binding site of the EBP-EMP1 complex. Due to the symmetrical nature of the complex, peptide-1 and peptide-2 have equivalent interactions with the two EBP molecules. The hydrogen bond interactions were analyzed using HBPLUS (McDonald et al., J. Mol. Biol. 238:777, 1994), based upon both distance (3.9 Å cutoff) and geometrical considerations.

A number of embodiments of the present invention have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the invention. Accordingly, it is to be understood that the invention is not to be limited by the specific illustrated embodiment, but only by the scope of the appended claims.

all.con	Thu	Apr 25	15:08:07 1996	1									
EBPI	EBP1-PEPTIDE1												
VDW	1 LEU 33		4 PHE 308 CE1 1	3.95									
VDW VDW	1 LEU 33	CB .	4 PHE 308 CD1 1	4.11									
VDW VDW	1 PHE 93 1 PHE 93	CE1	4 TRP 313 CH2 1 4 TRP 313 CH2 1	3.74									
VDW	1 PHE 93	.CZ	4 TRP 313 CH2 1 4 TRP 313 CZ2 1	3.98 4.08									
VDW	1 PRO 149	CA	4 GLY 309 0 1	3.59									
VDW VDW	1 PRO 149 1 PRO 149	CB	4 GLY 309 0 1	3.49									
VDW	1 MET 150	C N	4 GLY 309 0 1 4 PRO 310 0 1	3.66									
VDW	1 MET 150	N	4 PRO 310 0 1 4 PRO 310 C 1	3.35 3.62									
VDW	1 MET 150	CA	4 LEU 311 0 1	3.41									
VDW VDW	1 MET 150 1 MET 150	CA CA	4 GLY 309 0 1	3.78									
VDW	1 MET 150	CG	4 LEU 311 C 1 4 PHE 308 CD2 1	3.87									
VDW	1 MET 150	CG	4 PHE 308 CB 1	3.50 3.70									
VDW	1 MET 150	CG	4 PHE 308 CG 1	3.79									
VDW VDW	1 MET 150 1 MET 150	SD	4 PHE 308 CD2 1	3.52									
VDW	1 MET 150	SD SD	4 THR 312 C 1 4 THR 312 CA 1	3.55									
VDW	1 MET 150	SD	4 THR 312 CA 1 4 TRP 313 N 1	3.58 3.75									
VDW	1 MET 150	SD	4 PHE 308 CA 1	3.73									
VDW	1 MET 150	SD	4 PRE 308 CB 1	4.03									
VDW VDW	1 MET 150 1 MET 150	CE CE	4 PHE 308 CD2 1 4 TRP 313 CE2 1	3.45									
VDW	1 MET 150	CE	4 TRP 313 CE2 1 4 PHE 308 CE2 1	3.71									
VDW	1 MET 150	CE	4 TRP 313 CD2 1	3.79 3. 8 3									
VDW	1 MET 150	CE	4 TRP 313 NE1 1	3.91									
VDW VDW	1 MET 150	CE	4 TRP 313 CZ2 1	4.10									
VDW	1 MET 150 1 THR 151	C N	4 LEU 311 0 1 4 LEU 311 0 1	3.41									
VDW	1 THR 151	CA	4 LEU 311 0 1 4 PRO 310 0 1	3.45									
VDW	1 THR 151	CB	4 PRO 310 0 1	3.82 3.56									
VDW	1 THR 151	OG1	4 LEU 311 CD2 1	3.43									
VDW VDW	1 THR 151 1 THR 151	0G1	4 LEU 311 CA 1	3.91									
VDW	1 SER 152	CG2 CB	4 PRO 310 0 1 4 LEU 311 0 1	3.60									
VDW	1 HIS 153	NDI	4 LEU 311 0 1 4 LEU 311 0 1	3.54 3.57									
SHORTVDW	1 HIS 153	CE1	4 THR 312 OG1 1	2.87									
. ADM . ADM	1 HIS 153 1 HIS 153	CE1	4 THR 312 CB 1	3.48									
VDW	1 HIS 153	CE1 NE2	4 THR 312 CA 1 4 THR 312 OG1 1	3.76									
VDW	1 PHE 205	CE2	4 THR 312 OG1 1 4 PHE 308 CZ 1	3.57 3.90									
VD#	1 PHE 205	CZ	4 PHE 308 CE2 1	3.40									
VDW E	1 PHE 205	CZ	4 PHE 308 CZ 1	3.53									
VDW	BP2-PEP1 .2 SER 591	CA	4 TYR 304 OH 1	3 44									
VDW	2 SER 591	CB	4 TYR 304 OH 1	3.44 3.88									
VDW	2 SER 591	CB	4 PRO 317 CB 1	3.95									
VDW .	2 SER 591 2 SER 591	OG OG	4 TYR 304 OH 1	3.44									
VDW	2 SER 591	og og	4 PRO 317 CB 1 4 TYR 304 CZ 1	3.61									
VDW	2 SER 591	OG	4 TYR 304 CZ 1 4 TYR 304 CE2 1	3.83 3.84									
VDW	2 SER 591	C	4 TYR 304 OH 1	3.62									
VDW	2 SER 592	N	4 TYR 304 CE2 1	3.66									
VDW VDW	2 SER 592 2 SER 592	N CA	4 TYR 304 CZ 1	3.68									
VDW	2 SER 592	CB	4 TYR 304 OH 1 4 TYR 304 OH 1	3.80									
VDW	2 SER 592	c	4 TYR 304 CE2 1	3.73 4.00									
VDW	2 SER 592	0	4 TYR 304 CE2 1	3.53									
ADM ADM	2 SER 592 2 PHE 593	O.	4 PRO 317 CD 1	3.59									
VDW	2 PHE 593	CB CD1	4 CYS 315 O 1 4 CYS 315 CB 1	3.74									
VDW	2 PHE 593	CD1	4 CYS 315 CB 1 4 TYR 304 CD2 1	3.55 3.72									
				3.12									

all.com	Thu Apr 25	15:08:07 1996	2	
VDW 2 VDW 2 SHORTVDW 2	PHE 593 CE1 VAL 594 CG1	4 TYR 304 CE2 4 CYS 315 CB 4 PRO 317 CG	1 1 1	3.90 3.71 3.17 3.23
SHORTVDW	VAL 594 CG1	4 PRO 317 CD		3.23
	-PEPTIDE2 .CB	4 PRO 417 CB	1	3.84
1211	1 SER 91 CB	4 PRO 417 CG	1	3.90 3.90
VDW	1 SER 91 OG	4 PRO 417 CB 4 TYR 404 CE2	1	3.82
V 2	1 SER 92 N 1 SER 92 CA	4 TYR 404 OH	ī	3.85
12	1 SER 92 CA 1 SER 92 CB	4 TYR 404 OH	1	3.42
VDW	1 SER 92 CB	4 TYR 404 CZ 4 TYR 404 CE2	1	4.04 4.09
NDM	1 SER 92 CB 1 PHE 93 CB	4 TYR 404 CE2 4 CYS 415 O	î	3.43
VDW	1 PHE 93 CB 1 PHE 93 CD1	4 TYR 404 CE2	1	3.71
· VDW	1 PHE 93 CD1	4 TYR 404 CD2	1	3.83 3.92
VDW	1 PHE 93 CD1	4 CYS 415 CB 4 CYS 415 CB	1	4.08
VDW	1 PHE 93 CE1 1 PHE 93 CE1	4 CYS 415 CB 4 TYR 404 CE2	ī	4.09
VDW VDW	1 PHE 93 CE1 1 VAL 94 CG1	4 PRO 417 CG	1	3.54
VDW	1 VAL 94 CG1	4 PRO 417 CD	1	3.54 4.11
VDW	1 VAL 94 CG2	4 PRO 417 CG	1	4.11
	-PEPTIDE2 2 LEU 533 CB	4 PHE 408 CE1	1	3.14
SHORTVDW VDW	2 LEU 533 CB 2 LEU 533 CB	4 PHE 408 CD1	1	3.77
VDW	2 LEU 533 CB	4 PHE 408 CZ	1	4.00 4.05
VDW	2 LEU 533 CG	4 PHE 408 CE1 4 PHE 408 CE1	1	3.75
VDW	2 LEU 533 CD1 2 LEU 533 CD1	4 PHE 408 CE1 4 PHE 408 CZ	î	3.92
VDW VDW	2 LEU 533 CD1 2 LEU 533 O	4 PHE 408 CE1	1	3.67
VDW VDW	2 PHE 593 CE1		1	3.34 3.41
VDW	2 PHE 593 CE1		1	3.41
VDW	2 PHE 593 CZ 2 PHE 593 CZ	4 TRP 413 CZ2 4 TRP 413 CH2	ī	3.96
VDW VDW	2 PHE 593 CZ 2 PRO 649 CA	4 GLY 409 O	1	3.79
VDW VDW	2 PRO 649 CB	4 GLY 409 O	1	3.56
VDW	2 PRO 649 C	4 PRO 410 O 4 PRO 410 O	1	3.72 3.59
VDW	2 MET 650 CA 2 MET 650 CA	4 PRO 410 O 4 GLY 409 O	î	3.67
ADM ADM	2 MET 650 CA 2 MET 650 CA	4 LEU 411 O	1	3.77
ADM.	2 MET 650 CG	4 PHE 408 CD2	1	3.80
VDW	2 MET 650 CG	4 PHE 408 CG 4 PHE 408 CB	1	3.92 4.05
VDW	2 MET 650 CG 2 MET 650 SD		ì	3.72
ADM ADM	2 MET 650 SD 2 MET 650 SD		1	3.75
VDW	2 MET 650 SD	4 PHE 408 CD2	1	3.76 3.78
VDW	.2 MET 650 SD		1 1	4.02
VDW	2 MET 650 SD 2 MET 650 CE		ī	3.67
VDW VDW	2 MET 650 CE 2 MET 650 CE	4 TRP 413 NE1	1	3.76
VDW	2 MET 650 CE		1	3.76 3.83
VDW	2 MET 650 CF		1	3.88
VDW	2 MET 650 CE 2 MET 650 CE		ī	3.89
VDW VDW	2 MET 650 CI 2 MET 650 CI	4 TRP 413 CG	1	3.90
VDW	2 MET 650 C	4 LEU 411 O	1	3.54 3.57
VDW	2 MET 650 C	4 PRO 410 O 4 LEU 411 O	1	3.56
VDW	2 THR 651 N 2 THR 651 N		ī	3.77
VDW VDW	2 TER 651 C	A 4 PRO 410 O	1	3.41
SHORTVD	W 2 THR 651 C		1	3.03 3.98
VDW	— ———————————————————————————————————	B 4 PRO 410 C B 4 LEU 411 CA	1	4.02
VDW VDW		G1 4 PRO 410 C	ī	3.62

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VDW	2	SER	652	N	4	LEU	411	С	1	3.83
VDW	2	SER	652	CA	4	LEU	411	ŏ	î	3.51
VDW	2	SER	652	CB	4	LEU	411	ŏ	ī	3.18
VDW	2	SER	652	CB	4	LEU	411	č	ī	4.09
VDW	2	SER	652	OG.	4	THR	412	CB	ī	3.73
SHORTVDW	2	HIS	653	.CE1	4	THR	412	OG1	ī	3.00
VDW	2	HIS	653	CE1	4	THR	412	СВ	ī	3.91
PEPTIDE1-PEPTIDE2										
SHORTVDW	3	THR	303	OG1	4	HIS	407	CB	1	2.94
VDW	3	THR	303	OG1	4	HIS	407	CA	1	3.61
VDW	3	TYR	304	CB	4	CYS	406	0	1	3.86
VDW	3	TYR	304	CD1	4	TRP	413	CZ3	1	3.81
VDW	3	TYR	304	CD1	4	TRP	413	CH2	1	3.94
VDW	3	TYR	304	0	4	CYS	406	N	1	3.33
VDW	3	TYR	304	0	4	CYS	406	0	1	3.47
VDW	3	TYR	304	0	4	SER	405	CA	1	3.57
VDW	3	SER	305	CA	4	TYR	404	0	1	3.51
VDW	3	SER	305	С	4	TYR	404	0	1	3.77
VDW	3	CYS	306	0	4	THR	403	CB	1	3.50
VDW	3	CYS	306	0	4	TYR	404	CB	1	3.54
VDW	3	CYS	306	0	4	TYR	404	CD1	1	3.59
VDW	3	CYS	306	0	4	TYR	404	CA	1	3.75
VDW	3	CYS	306	CB	4	CYS	406	SG	1	3.81
VDW	3	CYS	306	SG	4	CYS	406	SG	1	3.75
VDW	3	CYS	306	SG	4	CYS	406	CB	1	4.06
VDW	3	PHE	308	CEl	4	TYR	404	OH	1	3.93
VDW	3	PHE	308	CE1	4	TYR	404	CE1	1	4.08
VDW	3	TRP	313	CG	4	TRP	413	CD1	1	3.85
SHORTVDW	3	TRP	313	CD1	4	TRP	413	CD1	1	3.04
VDW	3	TRP	313	CD1	4	TRP	413	NE 1	1	3.37
VDW	3	TRP	313	CD1	4	TRP	413	CG	1	4.09
VDW	3	TRP	313	NE1	4	TRP	413	CD1	1	3.31
VDW	3	TRP	313	CZ2	4	CYS	415	SG	1	3.84
VDW	3	TRP	313	CH2	4	CYS	415	SG	1	3.83
VDW	3	CYS	315	SG	4	TRP	413	CZ2	1	3.59
VDW	3	CYS	315	SG	4	TRP	413	CE2	1	3.95
VDW	3	CYS	315	SG	4	TRP	413	CH2	1	4.00
VDW	3	GLN	318	CD	4	GLN	418	NE2	1	3.28
VDW	3	GLN	318	OE1	4	SER	405	CB	1	3.80

ATOM

ATOM

ATOM

MOTA

ATOM

66 CG LET

57

69

CD1 LEU

CD2 LEC

LEC

LEU

С

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18

18

Thu Apr 25 12:27:47 1996 bref21c.pdb THE COMPLEX BETWEEN THE EXTRACELLULAR DOMAIN OF ERYTHROPOIETIS REMARK RECEPTOR (EBP) AND AN AGONIST EPO MIMETIC PEPTIDE 1 (EMF1) REMARK **** WARNING **** RESIDUES 21-23 (521-523) and 164-166, 633-636 REMARK HAVE WEAK OR NO ELECTRON DENSITY MAP AND HAVE BEEN MODELED REMARK INTO THE STRUCTURE. THESE RESIDUES HAVE A HIGH B OF 90. REMARK REMARK THE STRUCTURE CONSISTS OF TWO RECEPTOR (RESIDUES 10-220, 510-720) REMARK AND PEPTIDE (RESIDUES 303-318, 403 418) MOLECULES.

1 N LYS 10 40.090 29.257 22.042 1.00 22.57 REMARK 10 MOTA 1 30.133 20.962 1.00 23.45 39.634 10 ATOM 2 CA LYS 38.753 29.361 19.979 1.90 22.87 10 MOTA 3 CB LYS 38.334 30.155 18.735 1.00 22.92 CG LYS 10 ATOM 4 29.212 17.552 1.00 24.27 10 38.119 5 CD 1.45 ATOM 28.015 17.890 1.00 26.55 37.165 10 ATOM 6 CE LYS 17.998 35.685 28.367 1.00 26.18 7 N2 LYS 10 ATOM 31.427 21.420 1.00 22.91 38.921 C LYS 10 MOTA 8 32.442 21.636 1.00 24.17 39.589 MOTA 9 0 LYS 10 1.00 21.40 31.386 21.640 37.602 MOTA 10 N PHE 11 32.588 22.026 36.868 1.00 13.56 PHE 11 ATOM 11 CA 32.257 22.725 1.00 19.07 PHE 11 35.549 12 CB MOTA 34.497 22.609 1.00 20.24 PHE 33.362 CG 11 MOTA 13 34.717 22.670 1.00 19.49 CD1 PHE 34.862 14 11 ATOM 1.00 19.51 33.038 22.400 CD2 PHE 33.142 ATOM 15 22.527 CE1 PHE 33.910 35.728 1.00 19.64 11 ATOM 16 22.257 1.00 20.10 32.180 34.041 17 CE2 PHE 1: ATOM ..00 19.48 22.321 18 CZ PHE 32.568 35.395 ATOM 1.00 19.32 22.887 PHE 11 37.644 33.56? ATOM 19 34.740 1.00 18.89 37.77E 22.516 MOTA 20 PHE 11 38.181 33.106 24.016 1.00 20.71 GLU ATOM 21 1.00 20.59 24.886 12 38.905 34.036 22 CA GLU ATOM 26.246 1.00 21.48 39.253 33.423 CB GLU 12 23 MOTA 27.123 1.00 23.60 CG 12 40.185 34.309 24 GLU ATOM 1.00 25.09 39.455 35.301 29.056 25 CD GLU 12 MOTA 40.024 36.417 28.275 26 OE1 GLU 12 ATOM 1.00 21.05 OE2 GLU 12 38.356 34.952 28.589 27 ATOM 24.172 1.00 19.22 40.137 34.539 GLU 12 28 С ATOM 40.513 35.703 24.334 1.00 18.49 GLU 12 ATOM 29 0 40.730 33.687 23.341 1.00 17.67 SER 13 MOTA 30 N 34.094 22.571 1.00 16.71 41.903 SEF. 13 ATOM 31 CA 32.898 21.851 1.00 18.51 42.522 MOTA 32 CB SER 13 1.00 23.19 42.256 32.959 20.459 MOTA 33 OG SEE 13 41.570 35.202 21.554 1.00 15.57 SER 34 С 13 MOTA 21.546 1.00 15.13 42.239 36.248 13 ATOM 35 0 SEF. 40.563 34.955 20.698 1.00 12.00 LYS 14 MOTA 36 N 8.51 40.117 35.912 13.675 1.00 37 CA LYS 14 ATOM 39.063 25.287 13.769 1.00 5.96 14 CB LYS MOTA 38 34.366 17.714 33.862 15.761 CG 39.629 1.00 2.36 LYS 14 39 MOTA CD 38.566 1.00 2.00 LYS 14 40 MOTA ...00 2.27 39.191 33.270 15.496 CE. LYS 14 ATOM 41 38.193 32.742 14.528 1.00 2.00 NZ LYS 14 ATOM 42 39.586 37.198 20.295 1.00 3.05 С LYS 14 MOTA 43 38.290 19.755 39.782 1.00 7.15 MOTA 44 0 LYS 14 38.920 37.053 21.442 1.00 11.98 ATOM 45 N ALA 15 38.375 38.188 22.194 37.571 37.697 23.378 1.00 12.13 46 CA ALA 15 MOTA 1.00 11.49 47 CB ALA 15 ATOM 1.00 12.49 38.960 22.666 39.592 MOTA 48 C ALA 15 22.535 40.189 ATOM 49 0 ALA 15 39.683 38.207 23.167 1.00 13.97 50 'N ALA 16 40.560 MOTA 41.792 38.796 23.615 1.00 14.37 MOTA 51 CA ALA 16 37.710 24.052 ..00 14.76 42.771 52 CB ALA 16 MOTA 1.00 15.45 42.361 39.56? 22.426 ALA 16 MOTA 42.624 40.759 22.537 1.00 15.35 0 16 MOTA ALA 38.896 21.274 17 1.50 15.12 42.444 ATOM 55 N LEU 43.007 39.467 20.042 1.00 15.92 ATOM 56 CÀ LEU 39.428 13.910 57 CF LET 43.012 1.00 15.72 ATOM CG 44.204 37.485 18.662 1.00 17.46 ATOM 58 45.474 38.294 18.506 1.00 15.45 CD1 LEU ATOM 59 13.774 1.00 16.32 MOTA 60 202 44.360 36.462 40.741 42.374 19.512 ATOM 61 42.985 41.433 1.00 15.31 o LE: 18.711 ATOM 41.136 41.013 19.908 1.06 17.34 N LEU 12 MOTA 63 42.210 19.443 40.434 .00 15.72 MOTA CA LEU 18 41.867 5.00 13.72 ATOM 65 CB LET 18 38.999 19.022

28.725 41.263

40.393 43.284

41.260

42.117

39.876 44.375 20.257

37.235

39.422

17.640

15.625

20.500

17.329

1.00 9.76 1.00 5.61

..00 10.13

1.06 17.38

..00 19.32

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MOTA	71	N	ALA	19	40.92	42.981	21.680	1.00 19.88	;
MOTA	72	CA	ALA	19	40.92		22.789		٤
MOTA	73	CB	ALA	19	41.560	43.331	24.041		6
MOTA	74	С	ALA	19	41.60	45.273	22.445		ε
ATOM	75	0	ALA	19	42.02		21.294	1.00 25.03	3
MOTA	76	N	ALA	20	41.64		23.453		7
ATOM	77	CA	ALA	20	42.24		23.333		Ó
ATOM ATOM	78 79	CB	ALA	50.	41.52		24.310		6
MOTA	80	С 0	ALA ALA	20 20	43.77(23.562		ē
ATOM	81	N	ARG	2:	44.32		23.505 23.848		ŧ
ATOM	82	CA	ARG	2:	45.76		24.075		5
ATOM	83	CB	ARG	21	46.56		22.819		6
MOTA	84	CG	ARG	21	45.B2		21.446		5
ATOM	85	CD	ARG	21	45.71		20.863		6
MOTA	86	NE	ARG	21	44.76		21.591		7
ATOM	87	cz	ARG	21	43.441		21.610		6
ATOM	88		ARG	21	42.91		20.926		7
atom atom	89 90	C	ARG ARG	21 21	42.669 46.29		22.350		7
ATOM	91	ò	ARG	21	45.87		24.590 24.132		5
ATOM	92	N	GLY	22	47.15		25.614		8 7
ATOM	93	CA	GLY	22	47.82		26.193		5
ATOM	94	C	GLY	22	49.05		25.314		ó
MOTA	95	0	GLY	22	48.93		24.089		3
atom	96	N	PRO	23	50.23	51.765	25.872		7
ATOM	97	αD	PRO	23	50.31		27.119	1.00 90.00	ó
ATOM	98	CA	PRO	23	51.45		25.062		ó
ATOM	99	CB	PP.O	23	51.71		25.287		5
MOTA MOTA	100 101	CC	PRO PRO	23 23	51.52° 52.68°		26.850		ś
ATOM	102	Ö	PRO	23	52.56		25.544 26.123		ج. 3
ATOM	103	N	GLU	24	53.86		25.368		3 7
ATOM	104	CA	GLU	24	55.13		25.741		ó
MOTA	105	CB	GLU	24	56.33		25.238		6
MOTA	106	CG	GLU	24	56.47	9 52.149	23.723		6
MOTA	107	CD	CLU	24	56.71	50.822	22.959	1.00 24.22	6
MOTA	108		GLU	24	57.17		21.793		S
MOTA	109		GLU	24	56.43		23.478		5
MOTA MOTA	110	C	GLU	24	55.11		27.268		6
ATOM	111	0 N	GLU	24 25	54.87 55.34		27.829 27.925		3
ATOM	113	CA	GLU	25	55.37		29.377		7 5
ATOM	114	СВ	GLU	25	53.96		29.907		6
ATOM	115	CG	GLU	25	53.78		31.410	1.00 22.21	ó
ATOM	116	CD	GLU	25	53.19		21.799	1.00 27.17	÷
ATOM	117	OE1		25	53.46		31.057	1.00 27.15	ā
ATOM	118		GLU	25	52.46		32.837	1.00 26.11	3
MOTA	119	C	GLU	25	56.24		29.725	1.00 11.99	÷
atom atom	120 121	O N	GLU	25 26	56.05 57.24		29.181 30.572	1.00 14.38	3 7
ATOM	122	CA	LEU	26	58.14		21.001		ŗ
ATOM	123	CB	1.5	26	59.39		31.652		÷
ATOM	124		LEU	26	60.71		31.488		÷
ATOM	125	CD1	LEU	26	61.53	7 48.145	32.704	1.00 4.41	÷
MOTA	126		LEU	26	60.53		21.317	1.00 2.00	÷
ATOM	127	C	LES	26	57.40		22.030	1.00 6.68	•
MOTA		. 0	LZC	26	56.95		23.041	1.00 9.43	3 7
atom atom	129 130	N CA	LEU	27 27	57.31 56.61		21.797	1.00 5.17	•
ATOM	131	CB	LEU	27	55.42		32.035	1.00 5.71 1.00 6.50	:
ATOM	132	SG	LEU	2	54.28		21.673	1.00 10.34	•
ATOM	133		LET	2~	53.10		31.125	1.00 10.81	Sherry on the she
ATOM	134	CD2	LEU	27	53.87		32.906	1.00 7.08	÷
ATOM	135	τ	TE:	27	57.45	4 43.923	33.397	1.00 7.41	:
ATOM	136	Û	LEU	27	58.00		32.742	1.00 7.62	3
ATOM	137	N	CYS	58	57.46		34.726	1.00 7.42	
ATOM	138	CA	CYS	28	58.20		35.554	1.00 4.67	:
atom atom	139 140	0	CYS	28 28	57.24		36.529	1.00 4.38	-
ATOM	141	CB	CYS	28	56.21 59.26		35.861 36.357	1.00 2.56 1.00 3.64	:
ATOM	142	SG	CYS	28	60.42		35.358		: 6
ATOM	143	14	PHE	23	57.59		35.977	1.00 2.00	
ATOM	144	CA	Säī	29	56.81		37.943	1.00 2.00	٠
ATOM	145	CB	PHI	25	55.47	14 39.899	37.322	1.00 4.36	:
ATOM	146	CG	SHE	29	55.58		36,437	OC 3.43	•
MOTA MOTA	147 148		L PHE PHE	29	55.49		25.990	1.00 2.00	•
*** 47.1	740		. FAL	29	55.79	9C 38.747	25.058	1.00 2.30	

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ATOM	149	CE1		29		5.60		6.243	36.206	1.00	2.00	÷
MOTA	150	CE2		29		5.90		7.616	24.266	1.00	2.00	ę.
MOTA	151	CZ	PHE	29		5.81		6.365	34.843	1.00	3.80	•
MOTA	152	5	PHE	29 29		7.67 8.70		9.260 8.897	27.957	1.00	2.00	į
ATOM	153 154	о 0	PHE THR	30		7.34		8.814	39.766	1.00	4.17	7
atom Atom	155	CA	THP.	30		8.02		7.694	40.463	1.00	3.12	÷
ATOM	156	CB	THF.	30.		8.72		8.116	41.820	1.00	2.00	é
ATOM	157		THR	30	:	9.33	37 3	36.982	42.408	1.00	2.00	3
ATOM	158		THP.	30	:	57.76	_	36.661	42.827	1.00	2.00	5
ATOM	159	С	THP	30		6.95		36.601	40.674	1.00	6.81 8.70	é 3
ATOM	160	0	THR	30		55.77		36.924	40.814	1.00	7.95	7
MOTA	161	N	GLU	31		57.34 56.37		35.326 34.219	40.786		8.18	٤
MOTA	162	CA CB	GLU	31 31		56.5		33.240	39.650		7.89	6
atom Atom	163 164	CG	GLU	31		56.49		33.821	38.286		8.99	6
ATOM	165	CD	GLU	31		56.6		32.750	37.248		10.58	6
MOTA	166	OE1	GLU	31		57.5		32.875	36.395		13.03	3 3
MOTA	167		GLU	31		55.9		31.753	27.302		14.01 8.38	6
ATOM	168	C	GLU	31		56.4		32.432 32.940	42.079		9.7B	ě
MOTA	169	0	GLU ARG	31 32		55.4. 57.6		33.064	42.41		7.19	7
MOTA	170 171	N CA	ARG	32		58.0		32.390			8.64	÷
atom atom	172	CB	ARG	32		58.0		31.154		1.00	9.16	5
ATOM	173	CG	ARG	32		58.2		30.364	42.26		10.75	Ś
ATOM	174	CD	ARG	32		58.3	76	28.894			11.21	5
ATOM	175	NE	ARG	32		57.0		28.271			13.52	7
ATOM	176	CZ	ARG	32		56.3		28.350			16.55	გ 7
ATOM	177		ARG	32		56.7		29.036			17.12 17.67	7
ATOM	178		2 ARG	32		55.1		27.734 33.536			9.21	6
ATOM	179	c	ARG ARG	32 32		58.8		34.526		0 1.00	13.37	8
MOTA MOTA	180 181	о И	LEU	33		59.3		33.499				7
ATOM	182	CA		33		60.0		34.736		6 1.00		5
ATOM	183	CB		33		59.5	536	35.403				6
MOTA	184	CG		33		58.3		36.310				6
ATOM	185		1 LEU	33		57.0		35.584				6 6
ATOM	186		2 LEU	33		58.3		37.604				ě
ATOM	187	c	LEU	33 33		61.6		35.70			10.67	â
ATOM	188 189	O N	LEU GLU	34		62.		34.17				7
atom atom	190	CA		34		63.		34.21			8.09	6,
ATOM	191	CB		34		64.		32.00	5 44.73		10.89	5
ATOM	192	CG	GLU	34		63.		31.93			18.21	5
MOTA	193			34		62.		30.85			21.61	5 8
MOTA	194		1 GLU	34			810	30.22			22.26	3
ATOM	195		2 GLU	34			082 678	30.64 34.23				ě
ATOM	196		GLU GLU	34 34			413	33.45			0 10.91	•
ATOM	197 198		· ASP	35			978	35.15				7
ATOM ATOM	199			35			981	35.24			0 4.88	ક
ATOM	200			35			215	34.03		95 1.0	0 5.00	€.
MOTA	201			35	5		678	34.18				6
ATOM	202	2 01	D1 ASP	2:			.055	34.54				.
ATOM	203		D2 ASP	3.5			. 102	23.91				
MOTA	204			3:			.336 .563	36.56 37.19				
ATOM	205			3: 3:			. 677	37.0				
MOTA MOTA	20°			3			.098					÷
ATOM	20		B LEU				. 903					÷
ATOM	20		G LEU	3		62	. 21 9					
ATOM	21		D1 LEU	3	6		. 994					
ATOM	21		D2 LEU				.184					
MOTA	21		LEU		6		.119					
ATOM	21				6		.071					
ATOM	21				2		.038					
MOTA	21		A VAL		 		.960 .866					
ATOM	2i 21		:9 VAL :G1 VAL				.007					
MOTA MOTA	21		IGI VAL		-		. 957		-			
ATOM	21				,-		. 555		70 34.	329 i.	oc 3.89	9 -
ATOM	22		. VAL	. 3	7	59	.736	40.5			00 5.6	
ATOM	22	21 :	S CYS	3	8		.204					
ATOM			CA CYS		BE		1.831					
ATOM			5 578 5 67 8		38 38).762 L.592			715	00 5.14 00 8.4	
MOTA MOTA			O CYS OB CYS		38		1.801				00 2.9	
					38		1.86				00 3.2	
ATOM	2:	26	sa cy:	:	P C	61	1.B60	U 43	963 CA.	y . Z	UC 3.2	

bref2	lc.p	ďЪ		Thu	Apr 25 1	2:27:4 [.]	7 1996		4	
ATOM	227	N	PHE	39	59.811	42.540	30.742	1.00	4.35	;
ATOM	228	CA	PHE	39	59.621	42.507	29.286	1.00		
ATOM	229	CB	PHE	39	58.865	41.225	28.900	1.00		
ATOM ATOM	230	CC	PHE	39	57.461	41.198	29.411	1.00		
ATOM	231 232		PHE	39	56.416	41.686	28.636	1.00		Ŧ.
MOTA	233		PHE	39 39	57.190 55.123	40.807	20.709	1.00		5
ATOM	234		PHE	39	55.896	41.795	29.153	1.00		•
ATOM	235	cz	PHE	39	54.868	41.411	31.228 30.451	1.00		:
ATOM	236	C	PHE	39	58.826	43.713	23.794	1.00		÷
ATOM	237	0	PHE	39	58.262	44.451	29.580	1.00	4.23	3
ATOM	238	N	TRP	40	58.837	43.926	27.490	1.00	3.45	=
ATOM ATOM	239 240	CA	TRP	40	58.084	44.996	26.846	1.00		÷
ATOM	241	CB	TRP	40 40	58.826	46.352	26.872	1.00	4.45	÷
ATOM	242		TRP	40	60.014 61.386	46.517 46.185	25.928	1.00	7.44	
ATOM	243	CE2		40	62.143	46.555	26.200 25.062	1.00	9.31	5
ATOM	244	CE3	TRP	40	62.049	45.595	27.294	1.00	6.04 10.26	5 5
ATOM	245		Trf	40	60.003	47.056	24.661	1.00	8.12	6
ATOM	246		TRP	40	61.277	47.387	24.144	1.00	6.99	7
ATOM ATOM	247		TRP	40	63.527	46.358	24.989	1.00	10.83	Ð
ATOM	248 249		TRP TRF	40	63.431	45.395	27.217		10.6:	÷
ATOM	250	C	TRP	40 40	64.152 57.785	45.780	26.068	1.00		÷
ATOM	251	Õ	TRP	40	58.530	44.539	25.418	1.00	5.55	÷
ATOM	252	N	GLU	41	56.625	44.914	24.824 24.914	1.00	4.51	:
ATOM	253	CA	GLU	41	56.267	44.533	23.556	1.00	7.38 8.54	
MOTA	254	CB	GLU	4:	54.898	42.840	23.555	00	7.91	÷
ATOM	255	CG	GLU	41	54.860	42.586	24.450		11.7	÷
atom Atom	256 257	CD	GLU	41	53.619	41.687	24.254	1.00	13.67	÷
ATOM	258		GLU	41 41	53.418	40.748	25.055	1.00	15.11	3
ATOM	259	C	GLU	41	52.843 56.335	41.891 45.715	23.301	00	17.90	3
ATOM	260	ō	GLU	41	56.456	46.888	22.558 22.956	1.00	9.08	5
ATOM	261	N	GLU	42	56.403	45.389	21.271	1.00	8.71 8.40	3
MOTA	262	CA	GLU	42	56.426	46.399	20.211	1.00	9.64	5
ATOM	263	CB	GLU	42	57.729	47.207	20.227	1.00	6.56	6
ATOM	264	CG	GLU	42	58.974	46.393	20.511	1.00	5.93	4
ATOM ATOM	265	CD	GLU	42	60.242	47.114	20.115	1.00	7.51	•
ATOM	266 267	OE 2	GLU GLU	42	61.019	46.519	19.371	1.00	9.43	÷
ATOM	268	C	GLU	42 42	60.470 56.167	48.271	20.519	1.00	6.13	ē
ATOM	269	Š	GLU	42	55.88G	45.737 44.532	18.853	1.00	9.90	5
ATOM	270	N	ALA	43	56.243	46.514	18.795 17.771	1.00	9. 5 9 10.98	7
ATOM	271	CA	ALA	43	55.988	46.007	16.400	1.00	12.17	5
ATOM	272	CB	ALA	43	55.513	47.145	15.515	1.00	12.56	÷
ATOM	273	Ç	ALA.	43	57.164	45.291	15.731	1.00	10.71	÷
ATOM ATOM	274	0	ALA	43	58.309	45.583	15.930	1.00	12.40	÷
ATOM	275 276	N CA	ALA	44 44	56.87E	44.282	14.903	1.00	3.23	7
ATOM	277	CB	ALA	44	57.928 57.326	43.514	14.208	1.00	3.02	÷
ATOM	278	C	ALA	44	58.828	42.507 44.442	13.263	1.00	4.9	•
ATOM	279	ō	ALA	44	58.407	45.534	13.438 13.047	1.00	8.51	•
ATOM	280	N	SER	45	60.086	44.068	13.275	1.00	9.87 9.06	•
MOTA	281	CA	SER	45	60.962	44.325	12.508		10.3:	•
ATOM	282	CB	SER	45	61.616	46.002	13.354		11.34	
MOTA	203	OG.	SER	45	61.479	47.244	12.695		10.35	,
ATOM ATOM	284 ·		SER SEF	45	61.996	44.207	11.683	1.00	13.83	÷
ATOM	286	о И	ala	45 46	62.599 62.113	43.221	12.124	1.00	15.72	3
ATOM	287	CA	ALA	46	63.041	44.571 44.134	10.435 3.469	1.00	14.38	7
ATOM	288	CB	ALA	46	62.810	44.781	8.127	1.00	14.11	:
MOTA	289	С	ALA	46	64.379	44.538	10.028	1.00	15.43	:
ATOM	290	2	ALA	46	64.657	45.746	10.203	1.00	16.67	•
ATOM	291	N	GLY	47	55.140	43.525	10.433	00		-
atom Atom	292	CA	GLY	47	66.45C	43.762	11.009	1.00		:
ATOM	293 294	С 0	GLY.	47	66.558	44.415	12.400	1.00	15.13	•
ATOM	295	N	GLY Val	47 48	67.231 65.873	45.457	12.546	1.00	16.53	
ATOM	296	CA	AY:	48	65.950	43.843 44.302	13.399	1.00	:3.37	7
ATOM	297	CF	VAL	48	64.825	45.230	14.799 15.231	1.00	11.23	
ATOM	298	CG1	VA1	48	64.572	45.071	15.701	1.00	8.24 8.26	•
ATOM	299	CG2		48	65.216	46.556	14.964	1.00	6.13	:
ATOM	300	ć	VAL	48	65.904	43.069	15.642	. 00	3.65	
atom Atom	301	Ď.	VAL	48	65.062	42.183	15.443	1.00	9.93	;
ATOM	302 303	N CA	CT. CT.	49 49	56.882	42.949	16.521	00	3.48	-
ATOM	304	c	GLY	49	66.948 67.199	41.798 42.211	17.393	00	7.27	•
				-		70.611	13.829	1.00	5.14	÷

bref21	c.pdl	b		Thu	Apr	25	12	:27	:47	1996		5	
ATOM	305		SLY	49		7.29		43.3		19.152		3.06	5
ATOM	306		PRO	50		7.27		41.		19.732	1.00	4.49	7 8
ATOM	307		PRO	50		57.10		39.		19.536	1.00	2.00	ş
ATOM	308		PRO	5 C		57.51		41.		21.125	1.00	2.99	5
ATOM	309		PRO	50		57.54		40.		21.762	1.00	3.97 2.00	5
MOTA	310		PRO	50		57.9		39.		20.632 21.315	1.00	4.87	ş
ATOM	311		PRO	50		68.8		42		22.217	1.00	7.36	į
MOTA	312		PRO	50		68.94		43. 42.		20.403	1.00	5.60	7
ATOM	313		GLY	51		69.71 71.0		42.		20.477	1.00	2.83	Ŧ.
ATOM	314		GLY	51 51		70.9		44.		20.103	1.00	3.36	į.
MOTA	315		GLY GLY	51		72.0		44.		19.956	1.00	5.85	:
ATOM ATOM	316 317		ASN	52		69.7		44.		19.968	1.00	2.00	7
ATOM	318		ASN	52		69.6			211	19.604	1.00	2.00	5
ATOM	319		ASN	52		68.5			401	18.633	1.00	3.33	ક
MOTA	320		ASN	52		68.7	68	47.	534	17.666	1.00	7.97	ક
ATOM	321	OD1	ASN	52		69.2	33		311	16.538	1.00		ŝ
ATOM	322	ND2	ASN	52		68.4			753	18.079		10.05	7
MOTA	323	С	ASN	52		69.5			144	20.797	1.00	3.59	5
ATOM	324	0	ASN	52		69.5			359	20.638	1.00	2.00	5
MOTA	325	N	TYR	53		69.2			573	21.985	1.00	5.70	ė.
MOTA	326	CA	TYP.	53		69.1			350	23.229	1.00	5.58	5
MOTA	327	CB	TYP.	53		67.7			412	23.770	1.00	5.70	•
ATOM	328	ÇG	TYP.	53		66.6			. 547	22.768	1.00	4.84 6.02	ŧ
MOTA	329	CD1		53		66.0			. 414 . 495	22.188 21.282	1.00	5.48	ş
MOTA	230	CE1		53		66.1			.789	22.405	1.00	5.30	÷
MOTA MOTA	331 332		TYP. TYP.	53 53		65.1			. 891	21.495	1.00	6.56	è
ATOM	333	CZ	TYP.	53		64.5			.729	20.929	1.00	8.17	÷
ATOM	334	OH	TYF.	53		63.5			.767	19.987	1.00	12.54	3
ATOM	335	C	TYR	53		69.		46	. 667	24.308	1.00	3.83	ક
ATOM	336	Ó	TYR	53		70.		45	. 465	24.245	1.00	4.09	å
ATOM	337	N	SEP.	54		70.			.428	25.346	1.00	3.81	7
MOTA	338	CA	SEP.	54		70.			. 921	26.501	1.00	6.59	5
ATOM	339	CB	SER	54		72.			. 682	26.710	1.00	8.72	ě
MOTA	340	OG	SEP.	54		73.			.867	26.341		13.32	à .
atom	341	С	SER	54		70.			.035	27.726		4.52	ó
MOTA	342	0	SER	54		69.			.089	27.982		5.58	3
MOTA	343	N	PHE	55		69.			. 926	28.443		3.52	é
ATOM	344	CA	PHE	55		69.			.878	29.641		3.38 6.11	÷
MOTA	345	CB	PHE	55		68.			.676 .700			6.96	5
ATOM	346	CG	PHE	55		67. 65.			.865			10.17	4
ATOM	347		PHE	55 55			330		.547			8.73	÷
ATOM	348 349		PHE PHE	55			713		.879			12.64	ξ.
ATOM ATOM	250		PHE	55			317		.561			8.02	÷
ATOM	351	cz.	PHE	55			007		.728			8.93	÷
ATOM	352	c	PHE	55			942		.779		1.00	2.90	
ATOM	353	ာ	PHE	55		70.	476	44	.710	31.200	1.00	2.00	3
ATOM	354	N	SER	56		70.	083	46	5.892	31.595	1.00	2.00	-
ATOM	355	CA	SER	56			854		5.B62				•
MOTA	356	CB	SER	56			159		7.651				•
ATOM	357	OG	SER	56			950		B. 939				3
ATOM	358		SER	56			089		7.214				÷
ATOM	359		SER	56			080		7.943 6.635				;
MOTA	360		TYR	57			.546 .915		6.635 6.856				÷
MOTA	361		TYR	57 57			. 913 . 091		5.62				•
MOTA	362		TYR TYR	57			. 863		4.334				4
ATOM	363 364		1 TYR	57			. 254		3.83				÷
ATOM ATOM	365		1 TYR	57			. 865		2.58				4
MOTA	360		2 TYR	57			.115		3.56				÷
ATOM	36		2 TYR	5			. 729		2.31				•
ATOM	361			57	•		.09		1.83	4 37.26	0 1.00	2.00	
ATOM	36			•	-	71	. 673	2 4	0.59	1 37.33			:
MOTA	37		TYR	51			. 88		7.25		6 :.0	10.04	
ATOM	37	1 0	TYR	5			.09		7.18			11.97	
ATOM	37.		GLN	51			. 35		7.78			11.03	
MOTA	37			51			.18		8.14				
ATOM	37			5			. 61		19.59 in no			0 10.64	
ATOM	37			5			.16		50.09 51.43			0 13.28 0 13.57	
MOTA MOTA	37 37		GLN GLN	5 i			.16		52.43			0 13.57 0 15.62	
MOTA	37		2 GLN	5			.14		51.43			0 14.36	
MOTA	37		GLN				. 43		7.88				
ATOM	38		GLN				.48		48.58				
MOTA	38		LEU	5	ċ	70	7.77	7 4	46.79	e 41.70	59 1.0	0 8.41	- ا
MOTA	28				9	70	.18	3 4	46.43	5 43.03	36 1.C	C 6.4	3 -:

bref2	1c.p	£Ъ		Thu	Apr :	25 :	12:27:4	7 1996		6	
ATOM	383	СВ	LEU	59	70	. 534	44.993	43.313	1.00	4.10	ē.
ATOM	384	CC	LEU	59		. 811	44.344	44.446	1.00	2.46	5.
ATOM	385		LEU	59		.343		44.227	1.00	3.98	÷
MOTA MOTA	386 387	C	LEU LEU	59 50		. 246		44.462	1.00	6.03	5
ATOM	388	0	LEU	59 59		.926		43.995	1.00	9.36	5
ATOM	389	N	CLU	60		. 227		44.085 44.667	1.00	9.93	3 7
ATOM	390	CA	GLU	60		. 844		45.603		11.94	5
ATOM	391	CB	GLU	60		. 852	49.697	46.643		14.05	5
MOTA	392	CG	GLU	60	70	. 448		47.531		15.91	š
ATOM	393	CD	GLU	60		. 443		48.510		16.83	5
MOTA	394		CLU	60		. 263		49.607	1.00	16.52	ā
ATOM	395		GLU	60		.852		48.181		15.77	ŝ
MOTA MOTA	396 397	0	CTO.	60 60		.159 .200		46.315		14.73	6
ATOM	398	N	ASP	61		.193		47.189 45.973		14.00	8
ATOM	399	CA	ASP	61		.569		46.452		16.22 17.32	7 6
ATOM	400	CB	ASP	61		. 624		47.930		22.61	5
ATOM	401	CG	ASP	61	74	.287		48.814		26.60	5
ATOM	402		ASP	61		. 252		50.054	1.00	30.15	â
atom atom	403 404	C	ASP	61		.036		48.271		27.62	3
ATOM	405	Ö	ASP ASP	61 61		.390 .582		45.610		16.14	6
ATOM	406	N	GLU	62		.758	48.742 47.476	45.423 45.130		16.58	2 7
ATOM	407	CA	GLU	62		. 402	46.524	44.223		14.78 13.68	5
ATOM	408	CB	GLU	62		.418	45.359	43.931		15.90	5
ATOM	409	CG	GLU	62	74	. 592	44.612	42.585		20.15	÷
MOTA	410	CD	GLU	62		. 574	44.998	41.452		18.81	5
ATOM	411		GLU	62		. 324	46.202	41.202		19.09	8
ATOM	412		GLU	62		.047	44.078	40.788	1.00	17.28	3
ATOM ATOM	413	c	GLU	62		. 709	47.363	42.947		10.99	6
ATOM	414 415	o N	GLU PRO	62 63		.069 .744		42.704		11.23	3
ATOM	416	CD	PRO	63		. 785	46.984 45.973	42.173 42.435	1.00	9.01 9.66	7 6
MOTA	417	CA	PRO	63		.069	47.740	40.959	1.00	8.47	É
ATOM	418	CB	PRO	63		.517	47.322	40.691	1.00	5.33	5
MOTA	419	CG	PRO	63		. 504	45.895	41.103	1.00	7.09	6
ATOM	420	C	PRO	63		.146	47.407	39.779	1.00	6.19	5
ATOM ATOM	421 422	N	PRO	63		.473	46.366	39.775	1.00	4.91	8
ATOM	423	CA	TRP TRP	64 64		.119 .298	48.300 48. 09 2	38.788	1.00	3.37	7
ATOM	424	CB	TPP	64		.441	49.259	37.613 36.645	1.00	2.00	5 5
ATOM	425	CG	TP.P	64		. 591	50.490	36.923	1.00	2.40	5
MOTA	426	CD2	TRP	64		.181	50.651	36.67B	1.00	2.00	5
ATOM	427	CE2		64		. 845	51.972	27.050	1.00	2.28	÷
ATOM	428	CE3	TRP	64		.174	49.811	36.186	1.00	2.18	÷
atom atom	429 430		TP.P TP.P	54 54		.027 .995	51.682	37.410	1.00	2.00	5
ATOM	431		TPP	64		.537	52.573 52.476	27.487 36.950	1.00	2.00	7
ATOM	432		TPF	54		. 878	50.314	36.087	1.00	2.00 2.49	ę ę
ATOM	433		TRP	64		. 575		36.471	1.00	2.00	÷
MOTA	434	C	TP.F	64		.700		36.903	1.00	2.00	5
MOTA	435	2	TRP	64		. 677	46.528	26.736	1,00	2.00	3
ATOM	436	N	LYS	65		.704	46.036	36.524	1.00	2.00	7
atom atom	437 438	CA	LYS	65 65		. 909		35.803	1.00	2.00	5
ATOM	439	CG	TÄE	55 65		.603 .611	43.59? 43.306	26.668 37.673	1.00	2.61	•
ATOM	440		LYS	65		.207		38.401	1.00	3.35 4.33	5 6
ATOM	441	CE	LYS	55		.204	41.795	29.488		10.13	÷
ATOM	442	NZ	LYS	65	76	. 452	43.031	40.293		15.09	7
ATOM	443	c	LYS	55		.017	44.725	24.584	1.00	2.00	÷
atom Atom	444	3	275	55		.125		34.416	1.00	2.81	à
ATOM	445 446	SY %	LEC	56 56		.201	43.692	33.780	1.36	2.51	7
ATOM	447	25	LEU	÷5		.421	43.532	32.558	1.00	3.38	÷
MOTA	448	CG	LET	56		.135		21.340	1.00	2.07	÷
MOTA	449		LEU	56		.363		30.416	1.00	2.42 5.47	÷
ATOM	453		LEU	56		.327		30.383	1.00	2.99	5
ATOM	451	Ξ	LEU	66	72	. 651	42.234	22.492	1.00	3.16	•
ATCM ATOM	452	:	LET	56		.125		32.943	1.00	2.56	.3
MOTA MOTA	453 454	N	CYS	57		.479		21.885	1.00	4.64	:
ATOM	455	CÀ C	CYS	5 7 57		. 686		21.708	1.00	8.30	•
ATOM	456	õ	CYS	5. 57		.569		30.191	1.00	9.34	4
ATOM	457	CB.	CYS	57		.331		29.512 32.363	00	11.12	.d
MOTA	453	SG	CYS	5-		. 297		32.300	00	9.68 9.98	16
ATOM	459	2.	ARG	÷ŧ		. 672		29.649		10.38	• :
MOTA	460	CA	AP.G	68:		. 567		28.187		11.77	;

bref21	c.pd	Ь		Thu	Apr	25	12:	27:47	1996	7	
ATOM	461	СВ	ARG	68		71.38		8.359	27.627	1.00 15.15	:
ATOM	462	CG	ARG	68		72.36		8.376	26.053	1.00 20.38	ŧ.
MOTA	463	CD	ARG	68		71.85		7.102 5.943	25.359 25.653	1.00 25.20	-
ATOM	464	NE	ARG	68 68		71.0: 71.43		4.837	26.288	1.00 27.66	£
ATOM	465 466	CZ	ARG ARG	68		72.71		4.732	26.705	1.00 28.62	7
ATOM ATOM	467		ARG	68		70.60		3.818	26.498	1.00 27.68	•
ATOM	468	5	ARG	68.		69.14		9.327	27.751	1.00 9.76	•
ATOM	469	0	ARG	68		6B.44		8.504	28.317	1.00 9.75	•
ATOM	470	13	LEU	69		68.76		10.027	26.684	1.00 8.16	4
MOTA	471	CA	LEU	69		67.42		39.983	26.131	1.00 5.24 1.00 4.64	•
ATOM	472	C3	LEU	69		67.13		11.247 12.587	25.328 25.960	1.00 4.64 1.00 5.82	÷
MOTA	473	CG	LEU LEU	69 69		67.30		43.727	25.026	1.00 9.48	ę.
ATOM	474 475	CD1	LEU	69		66.49		42.773	27.111	1.00 9.06	÷
ATOM ATOM	476	c	LEU	69		67.22		38.794	25.221	1.00 6.45	÷
ATOM	477	Ö	LEU	69		68.17	15	38.217	24.655	1.00 6.60	3
HOTA	47B	N	RIS	70		65.94		38.430	25.133	1.00 6.17	•
ATOM	479	CA	HIS	70		65.44		37.374	24.296	1.00 4.34	Ę
MOTA	480	C3	HIS	70		64.75		36.308 35.494	25.103 25.871	1.00 3.32	÷
ATOM	481	CG	HIS HIS	70 70		65.7		34.706	25.460	1.00 7.46	į
MOTA MOTA	482 483		HIS	70		65.7		35.444	27.243	1.00 8.83	* - *
ATOM	484		HIS	70		66.7		34.653	27.650	1.00 9.22	÷
ATOM	485		HIS	70		67.3		34.193	26.586	1.00 6.78	
ATOM	486	С	HIS	70		64.4		30.097	23.546	1.00 6.62	•
MOTA	487	2	HIS	70		64.1		39.240	23.863	1.00 7.52	£
ATOM	488	N	GLN	71		63.8		37.453	22.520	1.00 10.06	:
ATOM	489	CA	GLN	71		62.8		36.038	21.676	1.00 12.44	1
MOTA	490	CB	GLN	71		63.4		39.628	19.675	1.00 12.33	į
ATOM	491 492	CD	gln Gln	71 71		63.1		40.157	18.423	1.00 11.98	÷
MOTA MOTA	493		GLN	71		63.2		41.364	18.185	1.00 14.18	£
ATOM	494		2 GLN	71		63.7		39.254	17.638	1.00 13.04	7
ATOM	495	С	GLN	71		61.8		36.915	21.278	1.00 14.54	÷
ATOM	496	0	GLN	71		62.2		35.846	20.828	1.00 13.15	:
ATOM	497	N	ALA	72		60.5		37.148	21.510	1.00 16.60	Ş
ATOM	498	CA	ALA	72		59.5		36.163 35.462	21.222 22.513	1.00 17.29	=
ATOM	499	CB C	ALA ALA	72 72		59.1 58.3		36.816	20.552		<u>.</u>
MOTA MOTA	500 501	Ö	ALA	72		57.9		37.949	20.890		3
ATOM	502	Ŋ	PRO	73		57.		36.140	19.535	1.00 15.70	
ATOM	503	CD		73		58.2	266	34.944	18.833		
ATOM	504	CA		73		56.		36.681	18.835		
MOTA	505			73		56.		35.789			
ATOM	506			73 73		57.1 55.3		34.500 36.586			
ATOM	507 508		PRO PRO	73		55.		35.678			
ATOM ATOM	509		THP.	74		54.		37.632			-
ATOM	510			74		53.		37.789	20.338		
ATOM	511			74		52.	987	39.276	20.518	1.00 3.94	
MOTA	512	CC	1 THR	74		54.		39.935			
MOTA	513		2 THR	74		51.		39.484			
ATOM	514		THR	74		52. 52.	216	37.289	19.382		
MOTA	515		THR ALA	74 75			237	36.542			
atom atom	516 517			75		30.		36.07			s - 6
ATOM	518			75			995	35.576	19.90	5 1.00 10.80) :
ATOM	51		ALA	75			612.			2 1.00 3.70) :
ATOM	52))		75			256	36.83		7 1.05 12.33	
MOTA	52			76			.583	38.41			
ATOM	52			76			107	39.55 40.78		6 1.50 10.91	, . A :
ATOM	52. 52			76			709	40.72			
MOTA MOTA	52			7			936	41.67		6 1.00 21.7	2
ATOM	52			7			.29€	41.16			
ATOM	52			7		47.	. 700	40.06		5 1.33 25.3	4
ATOM	52	8 N	H1 ARG	7			. 745	39.35		2 1.11 25.6	4 : 8 - 5 -
ATOM	52		H2 ARG	7			. 065			2 1.00 28.2	-
MOTA	53		ARG	7			.026				
MOTA	53 53			7			. 680 . 223				, -
MOTA MOTA	53		A GLY	· ÷			.121				
ATOM	53			7			.079			9 1.00 10.3	8
MOTA	53		GLY			53	. 633	41.81	4 15.10	2 1.00 10.5	
ATOM	53		ALA				.243			9 12.0	
ATOM	53		ALA				.158				
ATOM	53	8 (B ALA	. 7	ಕ	53	. 465	43.04	11 18.83	25 10.2	89

bref21	lc.pd	Ъ		Thu	Apr 25	12:27	7:47	1996		8	
ATOM	539	С	ALA	78	55.2	63 41	329	18.357	1.00	11.11	5
ATOM	540	0	ALA	78	55.0			18.495		13.01	ž
ATOM	541	N	VAL	79	56.4			18.640	1.00	9.69	7
ATOM	542	CA	VAL	79	57.5		178	19.192	1.00	7.22	5
MOTA	543	CB	VAL	79	58.8		_	19.354	1.00	6.05	5
MOTA MOTA	544 545		VAL	79	58.7			17.024	1.00	6.29	6
ATOM	546	C	VAL VAL	79 75	59.13 57.70			18.171 20.672	1.00	5.80	5
ATOM	547	ŏ	VAL	79	57.6			21.125	1.00	5.75 4.75	6 3
ATOM	548	N	ARG	8C	58.2			21.403	1.00	4.34	7
ATOM	549	CA	ARG	80	58.4			22.813	1.00	7.09	6
MOTA	550	CB	ARG	BO	57.5			23.550	1.00	8.65	3
MOTA	551	CG	ARG	80	57.4			25.052	1.00	7.34	5
atom Atom	552 553	NE NE	ARG ARG	8C 8C	56.6° 55.2°			25.630	1.00	6.89	ó
ATOM	554	cz	ARG	80	54.4			25.237 25.313	1.00	6.67 4.11	7
ATOM	555		ARG	80	54.8			25.743	1.00	5.04	7
MOTA	556	NH2	ARG	80	53.1			25.063	1.00	2.00	7
ATOM	557	С	ARG	80	59.8	46 40.	484	23.297	1.00	5.10	6
ATOM	558	0	ARG	80	60.4			23.114	1.00	3.87	9
ATOM	559	N	PHE	81	60.3			23.951	1.00	4.32	7
ATOM ATOM	560 561	CA CB	PHE PHE	81 81	61.6 62.3			24.488	1.00	5.56	6
MOTA	562	CG	PHE	81	62.7			24.305	1.00	4.97 5.07	6
ATOM	563		PHE	81	61.8			22.091	1.00	6.98	é
ATOM	564		PHE	ē:	63.9			22.409	1.00	7.17	6
MOTA	565		PHE	ā:	62.1		030	20.763	1.00	7.58	ક
MOTA	566		PHE	9:	64.2		908	21.086		10.89	6
ATOM	567	cz	PHE	ê: 0:	63.3			20.251		10.08	ó
ATOM ATOM	568 569	0	PHE PHE	81 81	61.5 60.7		209 848	25.955	1.00	7.23	6
ATOM	570	N	TRP	82	62.3		240	26.604 26.469	1.00	8.68 7.82	ō 7
ATOM	571	CA	TRP	82	62.2			27.891	1.00	8.83	દ
MOTA	572	CB	TRP	82	61.2		789	28.199	1.00	9.85	6
ATOM	573	CG	TRP	62	61.5		412	27.697	1.00	12.09	5
ATOM	574		TRP	82	62.2		372	28.428		11.52	6
ATOM ATOM	575 576		TRP TRF	82	62.3		248	27.577		13.27	E
ATOM	577		TRP	82 32	62.7 61.3		277 888	29.722 26.453		15.01 14.64	÷
ATOM	578		TRP	82	61.7		581	26.378		12.57	,
ATOM	579		TRF	82	62.9		048	27.987		17.05	5
ATOM	580		TRF	82	63.3		071	30.137		16.75	ē
MOTA	581	CH2	TRF.	82	63.4	15 33.	980	29.272	1.00	17.82	5
ATOM	582	C	TRP	82	63.6		561	28.371	1.00	8.05	6
ATOM ATOM	583 584	N N	TRP	82 83	64.6 63.7		733 156	27.623	1.00	7.22	3
ATOM	585	CA	CYS	83	65.0		749	29.635	1.00	7.16 5.52	? 6
ATOM	586	Ĉ.	CYS	33	64.6		373	31.702	1.00	4.93	÷
ATOM	587	0	CYS	83	63.7		969	32.271	1.00	5.95	å
ATOM	588	CB	CYS	33	66.0		909	30.319	1.00	7.79	é
MOTA	589	SG	CYS	83	66.4		538	31.992		15.35	15
atom atom	590 591	N CA	SER	84	65.2		353	22.258	1.00	3.11	7
ATOM	592	CB	SER SEF.	84 94	64.9 64.3		980 555	33.610 33.658	1.00	4.32	ş
ATOM	593	OG	SEP	54	65.0		752	32.731		12.40	3
ATOM	594	С	SEF.	84	66.1		135	34.483	1.00	7.36	÷
ATOM	595	0	SER	34	67.1	73 36.	544	34.190		11.62	÷ 7
ATOM	596		LEU	35	66.0		940	25.546	1.00	7.67	7
ATOM	597	CA	LEU	25	67.1		.209	36.457	1.00	4.28	5
MOTA MOTA	598 599	CB	LEU	85 35	66.6 66.7		160	37.546	1.00	3.56	÷
MOTA	600	CG	LEU	35	67.0		. 624 . 388	37.197 38.482	1.00	5.43	÷
ATOM	601		LEU	35	67.8		. 844	25.232	1.00		
ATOM	602	c	LEU	25	67.7		. 991	27.110	1.00		* * * *
MOTA	603	0	LEU	3.5	67.0	002 36.	. 021	2:.352	1.00		?
ATOM	604	N	PP.C	3.5	69.0		.01?	37.388	1.00		7
MOTA	605	CD	PRO	86	69.9		.092	35.989	1.00		÷
MOTA MOTA	606 607	CA CB	PRC- PRC-	30 86	69.1 71.2		.913 .361	38.036 37.921	1.00		4 4
MOTA	608	CG	PRO	3.5	71.2		.343	36.772	1.00		4
MOTA	609	ç	PPC	36	69.		.832	39.515	1.00		5
MOTA	610	0	PP.O	86	59.	142 36	.847	40.187	1.00	4.26	.3
MOTA	611	Ν.	THR	3.	69.		. 622	40.029	1.00		,
MOTA MOTA	612 613	CA CB	THR THR	27 87	68.		.399	41.394	00		:
ATOM	614		THR	8 · 8 *	68.9 68.9		.949 .183	41.727	1.00		÷
ATOM	615		THR	3-	68.		.599	42.975		11.56	.3
ATOM	616	С	THR	\$7	59.		.263	42.531	00		- 5

bref21	c.pdb	Thu Ap	x 25 12:2	7:47 1996	9
ATOM	617 O THR	g٦		.730 43.384	1.00 9.13
ATOM	618 N ALA	88		.474 42.541	1.00 8.99 T
MOTA	619 CA ALA	88		.286 43.568 .176 43.419	1.00 8.39 f
ATOM	620 CB ALA	88		.176 43.419 .752 43.497	1.00 8.97
ATOM	621 C ALA 622 O ALA	98 88		.573 44.247	1.00 10.83
ATOM	622 O ALA 623 N ASP	36		.090 42.578	1.00 8.36
atom atom	624 CA ASP	3 9.		.470 42.397	1.00 8.96
ATOM	625 CB ASP	6 3		.911 49.992	1.00 7.68
ATOM	626 CG ASP	89		.915 40.788	1.00 6.73 5 1.00 8.92 8
ATOM	627 OD1 ASP	89		.224 41.720 .646 39.667	
ATOM	628 GD2 ASP 629 C ASP	89 89		.746 42.654	1.00 9.65
MOTA	629 C ASP 630 O ASP	89		.880 42.522	1.00 9.22 3
atom atom	631 N THP	90		3.724 43.094	2.00 7.69
MOTA	632 CA THR	90		8.866 43.359	
MOTA	633 CB THP.	90		7.603 42.898	
MOTA	634 OG1 THR	90		5.466 43.495 7.445 41.430	
ATOM	635 CG2 THR 636 C THR	90 90		9.219 44.823	1.00 8.87 6
ATOM ATOM	636 C THR 637 O THR	90		8.790 45.335	1.00 11.62 5
ATOM	638 N SER	91		0.043 45.479	
ATOM	639 CA SER	91		0.434 46.87	
MOTA	640 CB SER	91		1.178 47.449 0.343 47.479	
atom	641 OG SER	97		0.343 47.470 1.265 47.03	
ATOM	642 C SER 643 O SER	91 91		2.197 46.26	3 1.00 9.93 8
atom	643 0 SER 644 N SER	92		1.029 48.12	5 1.30 8.52 7
ATOM ATOM	645 CA SER	92		1.671 48.33	
ATOM	646 CB SER	92		0.702 49.00	
ATOM	647 OG SER	92		0.120 48.08 2.992 48.96	
ATOM	648 C SER	92		12.992 48.96 13.499 48.74	· · · · · · · · · · · · · · · · ·
ATOM	649 O SER 650 N PHE	92 93		3.581 49.76	
MOTA MOTA	650 N PHE 651 CA PHE	93		4.847 50.36	6 1.00 3.55 6
ATOM	652 CB PHE	93		14.663 51.87	
ATOM	653 CG PHE	93		13.585 52.20	
MOTA	654 CD1 PHE	93		42.264 52.44	
MOTA	655 CD2 PHE	93		43.884 52.23 41.265 52.66	
ATOM	656 CE1 PHE	93 93		42.881 52.47	
MOTA MOTA	657 CE2 PHE 658 CZ PHE			41.573 \$2.70	04 1.00 2.00 🐔
ATOM	659 C PHE		63.923	46.107 50.0	
ATOM	660 O PHE	93		47.156 50.65	
ATCM	561 N VAL			46.008 48.93 47.054 48.43	
ATCM	662 CA VAI			46.501 48.2	
atom Atom	663 CB VAI 664 CG1 VAI			46.310 49.5	71 1.00 6.35 €
ATOM	665 CG2 VA		66.935	45.177 47.5	22 1.00 2.00 8
ATCM	666 C VA		65.042	47.525 47.0	
MOTA	667 O VA			46.793 46.3 48.780 46.6	
ATOM	668 N PR		65.364 65.947	48.780 46.6 49.823 47.5	
MOTA MOTA	669 CD PR		64.960	49.357 45.3	
ATOM	671 CB PR		65.316	50.826 45.5	30 1.00 2.93
atom	672 CG PR		65.261	51.036 47.0	
ATOM	673 C PR		65.783	48.756 44.2	
MOTA	674 · O PR		66.985 65.128	48.592 44.3	
MOTA	675 N LE 676 CA LE		65.776	47.852 41.5	
Mota Mota	677 CB LE		65.088	46.531 41.5	
ATCM	676 CG LE		65.571	45.607 40.	
ATOM	679 CD1 LE		66.945	45.060 40.	
ATOM	580 CD2 LE		64.648 65.713	44.446 40.3 48.886 40.	
ATOM	681 C LI 582 C LI		64.639	49.309 40.	
atom atom			66.881	49.355 40.	416 1.00 8.18
ATCM:		JU 97	67.000	50.324 39.	
ATOM	685 CB G	רָפּ טו	68.315	51.069 39.	
ATOM		יינ טו	68.162		849 1.00 10.56 676 1.00 12.04
ATOM		רכ טו רכ טו	67.806 68.087		73430 14.20
ATOM ATOM			67.252		691 1.30 17.02
ATOM		רק טו	66.959	49.610 27.	387 1.00 8.71
ATCH	s 691 ≎ G	LU 97	67.735		741 1.30 9.31
ATON		EU 38	66.083		.101 1.00 8.76 .821 1.30 3.77
ATOR		EU 98 EU 98	65.954 64.592		754 1.90 8.21
4OTA	4 694 CB L	EU 9R	34.332	40.033 00	

bref21	c.pc	D		Thu	Apr	25	12	: 27 : 47	1996		10	
ATOM	695	CG	LEU	98	6	4.36	6	47.487	35.606	1.00	9.97	÷
ATOM	696		LEU	98	6	2.91		47.080	35.721	1.00	9.15	Š
ATOM	697		LEU	98		5.20		46.309	35.266	1.00	3.89	Ę.
ATOM ATOM	698 699	0	LEU	98 98		6.14		50.388	24.676	00	9.74	5
ATOM	700	N	ARG	99		5.75 6.81		51.556 49.945	34.781 23.621		11.17	3
ATOM	701	CA	ARG	99		7.05		50.799	32.467	1.00	7.82 8.42	?
ATOM	702	CB	ARG	99		8.26		51.701	32.680	1.00	9.99	
ATOM	703	CG	ARG	99	6	8.31		52.571	33.915		13.57	ě.
MOTA	704	CD	ARG	99		9.54		53.483	33.832	1.00	15.63	•
ATOM	705	NE	ARG	99		0.79		52.717	33.766		21.42	7
atom atom	706 707	CZ	ARG	99 99		1.62 1.36		52.634	32.709		23.75	ż
ATOM	708		ARG	99		2.74		53.271 51.921	31.557		25.09 24.11	7
ATOM	709	C	ARG	99		7.29		50.002	21.174	1.00	7.84	5
ATOM	710	٥	ARG	99		8.17		49.159	31.118	1.00	8.53	ž
ATOM	711	N	VAL	100		6.52		50.307	30.136	1.00	5.56	7
MOTA	712	CA	VAL	100		6.67		49.664	28.852	1.00	5.54	ń
ATOM ATOM	713 714	CB	VAL	100 100		5.32 5.44		49.097	28.397	1.00	8.61	5
ATOM	715		VAL	100		4.82		48.467 48.100	27.008 29.419	1.00	7.63 7.70	÷ 5
MOTA	716	С	VAL	100		7.14		50.745	27.877	1.00	6.61	5
MOTA	717	0	VAL	100	6	6.55		51.831	27.819	1.00	3.63	•
MOTA	718	N	THR	101		8.23		50.490	27.156	1.00	7.98	7
ATOM ATOM	719 720	CA CB	THP.	101		8.76		51.483	25.193		10.18	ő
ATOM	721	0G1	THP.	101		0.00 0.52		52.277 51.629	26.748	1.00	8.43	÷
ATOM	722		THP.	101		9.60	_	53.663	27.908 27.148		13.91 11.20	÷
ATOM	723	C	THR	101		9.11		50.926	24.792		11.66	÷
ATOM	724	0	THR	101	6	9.48	3	49.758	24.645		11.61	ś
MOTA	725	N	ALA	102		8.91		51.752	23.767		12.50	7
atom atom	726 727	CA CB	ALA	102		9.21		51.369	22.306		14.07	÷
ATOM	728	C	ALA	102 102		B.73 0.72		52.465 51.154	21.399		14.73 13.24	5 5
ATOM	729	ŏ	ALA	102		1.51		51.752	23.012		12.22	8
ATOM	730	N	ALA	103		1.11		50.332	21.270		12.73	7
ATOM	731	CA	ALA	103		2.52		50.004	21.021	1.00	13.74	5
atom Atom	732 733	CB C	ALA	103		2.63		48.712	20.183		15.06	5
ATOM	734	Ö	ALA	103 193		3.25 3.95		51.173 51.013	20.33B 19.345		14.07	5
ATOM	735	Ň	SER	104		3.10		52.341	20.931		12.51	3
ATOM	736	CA	SEP.	104	7	3.67		53.569	20.440		10.25	÷
ATOM	737	CB	SEP	104		2.83		54.066	13.266	1.00	9.41	÷
ATOM ATOM	738 739	OG C	SER SER	104 104		1.43 3.50		54.033 54.528	19.565	1.00	8.47	3
ATOM	740	ŏ	SEP.	104		3.55		55.746	21.600		11.58	ŕ
ATOM	741	N	GLY	105		3.18		53.964	22.770		11.41	- 7
ATOM	742	CA	GLY	: 25		3.00		54.74?	23.976		12.64	÷
ATOM ATOM	743 744	0	GLY	105		1.73		55.568	23.980		13.51	•
ATOM	745	N	GLY	105 106		0.92		56.335 55.433	24.921		15.64	:
ATOM	746	CA	ALA	106		9.66		56.166	22.930 22.837		12.54	5
ATOM	747	EЭ	ALA	106		9.06		56.040	21.444		13.77	÷
ATOM	748	2	ala	106	6	B.75	2	55.553	23.884		11.28	÷
ATOM	749	0	ALA	196		8.50		54.338	23.899		10.70	5
ATOM ATOM	750 751	N CD	PRO PRO	107 107		8.23		56.392	24.779	1.00	a.60	:
ATOM	752		PRC	107		8.39		57.855 56.019	24.686 25.882	1.00	9.28 7.77	÷
ATOM	753	CB	PPC	127		7.28		57.314	25.683	1.00	8.42	-
ATOM	754	CG	PRO	197		7.30		58.358	25.605	1.00	9.15	+
ATOM ATOM	755	C	PRO	107		5.96		55.459	25.552	1.00	7.66	4
ATOM	756 757	0	PRO ARG	107 108		5.22 5.59		56.048 54.353	24.761	1.00	8.78	-
ATOM	758	CA	ARG	108		4.29		53.751	25.196 25.990	1.00	7.20	÷
ATOM	759	CB	ARG	108		4.43		52.415	25.288	1.00	7.43	
ATOM	760	CG	ap.g	108	6	3.16	68	51.903	24.695		10.88	4
MOTA	761	CD	ARG	108		2.76		52.688	23.460	1.00	14.12	•
atom atom	762 763	NE CZ	arg arg	108		1.46		52.313	22.964		15.25	:
ATOM	764		ARG	108 108		1.08 51.91		51.084	22.550 22.764		15.01	•
ATOM	765		ARG	108		9.8		50.867	22.236	1.50	18.31 19.47	?
ATOM	766	c	ARG	108		53.45		53.624	27.253	00		- 5
ATOM	767	÷.	AP.G	108		52.42		54.259	27.404	:.::	5.86	:
ATOM ATOM	768 769	N CÀ	TYR.	109 109		53.86		52.837	28.263	1.11		•
ATOM	770	CF	TYR	109		53.1(52.4)		52.711 51.350	29.509 29.631	1.20	4.72 7.62	•
ATOM	771	CG	TYP	109		51.45		51.024	23.544		3.20	•
ATOM	772	CD1	172	109		51.7		50.089	27.565		11.38	•

bref21	c.pdb	Thu 2	Apr 25 12	:27:47	1996	11	
ATOM	773 CE1 TYR	109				00 12.39	ė. E
ATOM	774 CD2 TYP.	109				00 10.61	Ę
ATOM	775 CE2 TYR	109				00 12.42 00 12.48	5
ATOM	776 CZ TYR					00 14.44	à
ATOM	777 OH TYR					00 8.52	5
MOTA	778 C TYR		65.124			00 9.59	\$
MOTA	779 O TYR		63.198		31.835 :.	00 10.99	7
MOTA MOTA	780 N HIS		63.760	53.467		00 14.45	•
ATOM	782 CB HIS	_	64.468			00 16.04	é
MOTA	783 CG HIS		65.167			00 21.12	÷
MOTA	784 CD2 HIS		66.383			.00 24.07	7
ATOM	785 ND1 HIS		64.623 65.476		36.662	.00 23.40	6
MOTA	786 CE1 HIS		66.553	55.114	36.321 :	.00 22.60	7
ATOM	787 NE2 HIS		62.628	53.380		.00 12.21	ć
MOTA MOTA	789 O HI		61.740	54.224		.00 13.06	B 7
ATOM	790 N AR		62.693	52.361		.00 11.08	ó
HOTA	791 CA AR		61.716	52.116 50.881		.00 10.30 .00 9.90	6
MOTA	792 CB AR		60.878 59.700	50.590		.00 8.05	5
MOTA	793 CG AR		58.370	50.465		.00 8.40	5
MOTA	794 CD AR 795 NE AR		57.828	49.099		.00 8.93	7
ATOM	795 NE AR 796 CZ AR		57.096	48.521	36.730	.00 8.80	÷
ATOM ATOM	797 NH1 AR		56.822	49.182		.00 10.13	7
ATOM	798 NH2 AR	_	56.585	47.308		.00 10.84	7
ATOM	799 C AR	G 111	62.546	51.850		00 11.27	ક 3
MOTA	800 C AF		63.776	51.808 51.758		.00 11.56	7
MOTA	801 N VA		61.877 62.493	51.471		.00 11.15	6
ATOM	802 CA VA		62.882	52.803		.00 12.50	5
MOTA	803 CB VJ 804 CG1 VJ		63.003	52.545		1.00 13.08	6
MOTA MOTA	805 CG2 VI		64.235	53.354		.00 12.31	6
ATOM		AL 112	61.398	50.668		1.00 7.77	5 3
ATOM		AL 112	60.269	51.105		1.00 5.20	7
MOTA		LE 113	61.709 60. 69 2			1.00 6.80	6
ATOM		LE 113 LE 113	60.223			1.00 5.60	6
ATOM			59.680		39.426	1.00 6.45	5
MOTA MOTA	811 CG2 I 812 CG1 I		61.396		40.315	1.00 7.39	5
MOTA	813 CD1 I	_	61.012	45.471	39.468	1.00 9.87	6
ATOM		LE 113	61.105		43.001	1.00 7.16	é
MOTA	815 C I	LE 113	62.141		43.572	1.00 9.02	7
MOTA		IS 114	60.267 60.503		43.4 6 3 44.645	00 2.00	5
ATOM		IS 114	59.793			1.00 2.00	5
ATOM		IIS 114	60.554	47.827	45.555	1.00 2.00	*
mota Mota	620 CD2 H		61.33			1.00 4.32	ş
ATOM	821 ND1 F		60.589			1.00 4.03	: •
ATOM	822 CE1 F		61.36			1.00 2.34	
MOTA	823 NE2		61.835 59.90			1.00 2.00	
MOTA		115 114				1.00 2.00	
ATOM		HIS 114 ILE 115				1.00 2.00	-
ATCM ATCM		ILE 115				1.00 2.00	
ATOM		ILE 115	61.43			1.00 3.84	
MOTA	829 CG2					1.00 4.23	
ATOM	830 · CC1					1.00 2.00	
ATOM	831 CD1					1.00 3.50	
MOTA		ILE 115				1.00 6.9	
MOTA		ILE 115 ASN 116	·	_		1.50 4.6	
ATOM		ASN 110				1.00 5.2	1 -
ATOM ATOM	835 CA 836 CB	ASN 11			2 43.370	1.00 5.3	
ATOM		ASN 11		82 43.82		1.20 5.9	
MOTA			6 59.4	70 44.42		1.00 8.0	
ATOM		ASN 11				1.00 8.4	
ATOM	840 C	ASN 11					
ATOM		ASN 11				1.00 8.3	
ATOM		GLU 11					
MOTA MOTA		GLU 11				1.00 6.3	1
ATOM		SLC 11	55.9	58 46.6	06 46.93~		
ATOM	846 CD	GLC 11	7 56.1			00 15.0	
ATOM	847 OE1	GLU 11					
ATON		GLU 11					
ATO		GLU 11					
ATO	1 8 50 3	GLU 11	54.4				

bref21	c.pc	ĪЬ		Thu	Apr	25 1	2:27:4	7 1996		12	
ATOM	851	N	VAL	118	55	5.477	43.151	43.523	1.00	3.55	;
ATOM	852	ÇA	VAL	118		5.226	42.839		1.00	2.91	•
ATOM	853	CB	VAL	118	56	5.373	43.488	41.261	1.00	2.00	:
MOTA	854		VAL	118		7.484	42.519	40.942	1.00	2.85	:
ATOM	855		VAL	118		5.828	44.165		1.00	2.00	÷
ATOM	856	C	VAL	118		5.060	41.334	41.948	1.00	2.18	•
ATOM	B57	O N	VAL	118		5.453	40.755	40.936	1.00	3.55	3
atom atom	858 859	CA	VAL VAL	119 119		1.404	40.716		1.00	2.79	:
ATOM	860	CB	VAL	119		4.155 3.776	39.276 38.736		1.00	3.05 2.45	:
ATOM	661	CG1		119		3.749	37.267	44.292	1.00	2.00	÷
MOTA	B62	CG2	VAL	119		1.735	39.231	45.352	1.00	2.00	
MOTA	863	¢	VAL	119	52	2.998	38.960		1.00	2.00	4
ATOM	864	0	VAL	119		2.007	39.674	41.932	1.00	2.00	3
ATOM	B65	N	LEU	120		3.171	37.919		1.00	3.02	7
ATOM ATOM	866 867	CA CB	LEU	120 120		2.175	37.411	40.174	1.00	2.95	÷
ATOM	868	CG	LEU	120		2.446 1.496	37.894 37.332	38.745 37.674	1.00	5.65	5
ATOM	869		LEU	120		0.125	37.938		1.00	9.95	5 5
ATOM	870		LEU	120		2.053	37.605	-		11.67	5
MOTA	871	С	LEU	120		2.289	35.887		1.00	2.40	- 5
ATOM	872	0	LEU	120	52	2.985	35.241	39.487	1.00	2.00	į
MOTA	873	ĸ	LEU	121		1.600	35.340		1.00	2.39	:
MOTA	874	CA	LEU	121		1.629	33.924		1.00	2.77	•
ATOM	875	CB	LEU	121		1.063	33.689		1.00	4.57	•
ATOM ATOM	876 877	CG CD1	LEU	121		2.050	33.227			10.24	•
ATOM	878	CD2		121 121		2.939 2.944	32.076 34.328			14.57	:
ATOM	879	c	LEU	121		0.974	32.995		1.00	9.45	:
ATOM	880	ō	LEU	121		0.256	33.420		1.00	5.41 7.90	₹ ₩
ATOM	881	N	ASP	122		1.279	31.709		1.00	8.57	7
ATOM	882	CA	ASP	122		0.687	30.726		1.00	6.90	÷
ATOM	883	CB	ASP	122		1.493	29.421	39.773	1.00	7.76	5
ATOM	884	CG	ASF	122		2.701	29.437		1.00	9.54	5
ATOM ATOM	685 686	OD1 OD2		122		2.927	30.429		1.00	9.98	5
ATOM	887	C	ASP	122 122		3.411 9.292	28.405 30.494			10.20	3
ATOM	888	ŏ	ASP	122		B.957	30.954	40.343	1.00	7.04 5.44	5
ATOM	889	N	ALA	123		B.464	29.813	29.568	1.00	6.22	7
ATOM	890	CA	ALA	123		7.107	29.562		1.00	4.75	÷
ATOM	891	CB	ALA	123	4	6.187	29.374	38.839	1.00	2.00	÷
MOTA	892	C	ALA	123		6.981	28.398		1.00	3.93	•
MOTA	893	0	ALA	123		7.826	27.484		1.00	5.37	•
ATOM ATOM	894 895	N CD	PRO	124		5.979	28.490		1.00	2.5:	7
ATOM	896	CY	PRO PRO	124 124		5.216 5.652	29.736 27.478		1.00	2.90	÷
ATOM	897	CB	PRO	124		4.362	28.022	-	1.00	2.91 2.55	÷
ATOM	898	CG	PRC	124		4.602	29.485		1.00	2.::	•
ATOM	899	С	PPC	124	4	5.451	26.111		1.00	2.00	÷
ATOM	900	0	PRO	124	4.	5.289	26.022	40.966	1.00	2.00	:
ATOM	901	N	VAL	125		5.524	25.042		1.00	2.21	
ATOM	902	A)	VAL	125		5.345	23.715		1.00	4.05	÷
ATOM ATOM	903 904	CGI	VAL VAL	125 125		6.724	23.006		1.00	2.01	-
ATOM	905		VAL	125		7.474 7.584	23.806 22.776		1.00	2.22	:
ATOM	906	c	VAL	125		4.436	22.838		1.00	2.00	
ATOM .	907	ō	VAL	125		4.002	23.281		1.00	5.51 6.33	:
ATOM	908		SLY	126		4.068	21.661		1.00	5.23	-
ATOM	909	CA	GLY	126		3.230			1.00		
ATOM	910	С	GLY	126		1.939			1.00		:
ATOM	911	O	GLY	126		1.588			1.00		:
MOTA MOTA	912	N	LEU	127		1.248			00		-
HOTA	913 914	CA CB	LEU	127 127		9.971 9.594	22.667		1.00		:
ATOM	915	CG	LEU	12-		8.175			1.00	3.12	:
ATOM	916		LEU	12-		7.954			1.00		:
ATOM	917		LEU	127		7.942				10.21	:
MOTA	918	C	LEU	12		8.846			1.00	6.31	
ATOM	919	0	LEU	12-	3	8.585	21.083	42.538	1.00	6.56	•
ATOM	920	N	VAL	125		8.177			1.00	7.03	:
atom atom	921 922	CA	VAL	128		7.087			1.00		•
ATOM	923		VAL	128 128		7.485			1.00		:
ATOM	924		VAL	128		7.999 8.521			1.00		•
ATOM	925	\$	VAL	128		5.862			1.00		: :
ATOM	926	Ü	VAL	126		5.973			1.00		
ATOM	927	N	ALA	129		4.691			1.00		:
ATOM	928	CA	ALA	129	3	3.430	21.061				÷

þı	ef21	c.pđ	b		Thu	Apr	25	12:	27:47	1996		13	
AT	'OM	929	СВ	ALA	129		2.58		1.680	44.477		4.36	5
	MO	930	c	ALA	129		2.69		9.876	46.202	1.00	9.11 9.32	3
	OM	931	0	ALA ARG	129 130		2.73 2.01	-	0.106	47.329	1.00	9.76	7
	MO:	932 933	N CA	ARG	130		1.28		9.020	47.990	1.00 1		ક ે
	COM	934	CB	ARG	130		32.22		8.310	48.967	1.00 1		é
	MO	935	CG	ARG	130		31.76		6.979	49.486	1.00 1		6 5
	MO1	936	CD	ARG	130		32.10 33.35		16.871 17. 5 67	50.963	1.00		ř
	MON	937	NE CZ	arg arg	130 130		33.66		18.135	52.414	1.00		÷
	M01 M01	938 939		ARG	130		32.81		18.092	53.449	1.00		7
	MOT	940		ARG	130		34.84		18.791	52.514	1.00		į
	TOM	941	c	ARG	130		30.02		19.479	48.721	1.00		5 8
	MOT	942	0	ARG	130		29.93		20.593 18.582	49.250 48.792	1.00		7
	TOM	943	N	LEU	131 131		29.0(27.8)		18.909	49.460	1.00		6
	TON	944 945	CA CB	LEU	131		26.6		18.313	48.688	1.00		6
	Tom Tom	946	CG	LEU	131		25.3		18.517	49.353	1.00		6
	TOM	947		LEU	131		25.0		20.002	49.487	1.00		6 6
	TOM	948		LEU	131		24.2		17.783	48.531 50.892	1.00	11.69	6
	TOM	949	c	LEU	131		27.7 27.7		18.409 17.204	51.128		12.81	à
	TOM	950	O N	LEU ALA	131 132		27.9		19.328	51.834		14.88	7
	TOM TOM	951 952	CA.	ALA	132		27.9		18.982	53.249		16.22	5
	TOM	953	CB	ALA	132		28.2		20.228	54.122		14.97	6
	TOM	954	С	ALA	132		26.6		18.324	53.656 54.109		16.57 16.97	.6 5
	TOM	955	0	ALA	132 133		25.7 26.5		19.000	53.411		20.15	7
	TOM	956 957	N CA	ASP ASP	133		25.3	_	16.156	53.729		22.27	5
	ntom Ntom	958	CB	ASP	133		25.8		14.755	54.193	_	23.23	6
	ATOM	959		ASP	133		26.1		12.783			25.72	5 3
	MOTA	960		1 ASP	133		25.7		14.012			26.91 25.03	3
	ATOM	961		2 ASP	133 133		26.6		12.758 16.814			22.10	6
	ATOM	962 963		ASP ASP			23.		17.415			24.05	8
	atom Atom	964		GLU			25.		16.802		7 1.00	19.91	7
	ATOM	965					24.	742	17.410			18.60	6
	ATOM	966		GLU	134		25.		16.953			17.36	5 5
	MOTA	967					26. 28.		15.897			17.83	6
	MOTA	968		GLU				980	15.726			19.82	ě
	atom Atom	969 970		2 GLU				136	17.775			18.81	3
	MOTA	97		GLU				784	18.933			17.19	ż
	MOTA	97		GL				842	19.534			18.37	9 7
	ATOM	97:		SE				375	20.93			17.66	÷
	MOTA MOTA	97. 97.						435	21.85			17.67	÷
	ATOM	97		_				623	21.98	1 55.40		19.35	•
	ATOM	97	7 C	SE	R 13	5		990	21.44			18.19	5
	ATOM	97		SĒ				. 366	22.50) 17.96) 19.82	
	ATOM	97						. 287 . 945	20.66 21.10			21.54	
	MOTA	98		k GL GL				.765	22.33			22.07	
	MOTA MOTA	98 98						. 225		5 51.93	0 1.0	22.69	-
	ATOM	98		_				.071	22.25	8 52.63		21.69	
	ATOM	98	4 C					. 992				0 19.69 0 22.11	
	ATOM	98						.594 .768				0 25.43	
	ATOM	98 98		G HI D2 HI				.049				0 27.18	
	MOTA MOTA	98		D1 H	_			.484				0 26.89	
	ATOM	98		E1 H			24	.014	26.28			0 26.67	
	MOTA	99	90 N	E2 H				. 944				0 26.59	
	ATOM	99						.081				0 20.00	
	ATOM		92 () H:				1.547				0 16.0	
	ATOM ATOM				AL 1			. 598				0 12.4) ÷
	ATOM				AL 1	8	28	3.391	24.1			0 12.4	
	ATOM	9	96 (G1 V		8.		72				00 10.70 00 12.9	
	MOTA			CG2 7.		28		?.444 9.89				00 12.9	
	MOTA					38 38		9.96				00 11.6	2 ;
•	MOTA	10				36 39		0.87			71 1.0	00 9.3	6 7
	ATOM					39	32	2.19	4 23.2			00 10.3	8 :
	ATOM	10	02	CB V	AL 1	39		2.53					
	ATOM			CG1 V		39		3.78					
	MOTA			CG2 V		39 39		1.41 3.24				00 10.0	
	MOTA MOTA					39		3.23				00 10.3	
	7. VI			•			-		-				

bref2	1c.pc	ь		Thu	Apr 25	12:27:47	1996	-	14	
ATOM	1007	N	LEU	140	33.975	24.194	49.372	1.00	a.25	;
ATOM	1008	ÇA	LEU	140	35.027		43.384	1.00	6.26	į.
ATOM	1009	CB	LEU	140	34.986		47.761	1.00	2.05	÷
ATOM	1010	CG	LEU	140	33.726	25.968	47.000	1.00	2.50	5
ATOM	1011	CD1	LEU	140	33.806	27.395	46.505	1.00	2.00	5
MOTA	1012		LEU	140	33.594		45.869	1.00	2.00	6
MOTA	1013	C	LEU	140	36.354		49.069	1.00	3.88	દ
ATOM	1014	0	LEU	140	36.566		50.115		10.60	ė
ATOM	1015	:i CA	ARG ARG	141	37.279		48.409		11.34	-
atom atom	1016 1017	CB	ARG	141 141	38.618 38.682		48.929 49.446		12.76	5
ATOM	1018	CG	ARG	141	39.347		50.793		16.99 21.35	5 5
ATOM	1019	CD	ARG	141	40.849		50.697		24.13	6
ATOM	1020	NE	ARG	141	41.431		52.042		29.12	7
ATOM	1021	CZ	ARG	141	42.344		52.482		30.00	6
MOTA	1022	NH1	ARG	141	42.821	23.266	51.673	1.00	30.75	7
ATOM	1023		ARG	141	42.727		53.773	1.00	29.95	7
ATOM	1024	C	ARG	141	39.632		47.804	1.00	13.10	6
ATOM	1025	0	ARG	141	39.289		46.639		13.55	3
ATOM ATOM	1026	N CA	TRP TRP	142 142	40.871		48.154		11.10	7
MOTA	1028	CB	TRP	142	41.754		47.182 46.354	1.00	6.61	5
ATOM	1029	CG	TRP	142	41.661		47.155	1.00	6.92 9.55	5 5
ATOM	1030		TPP	142	40.482		47.749	1.00	9.85	ŕ
ATOM	1031		TRP	142	40.852		48.397	1.00	9.31	5
ATOM	1032	CE3	TRP	142	39.145		47.788		10.67	ē
MOTA	1033	CD1	TRF	142	42.671	27.216	47.456	1.00	10.90	έ
ATOM	1034			142	42.196		48.209	1.00	11.52	7
ATOM	1035		TRF	142	39.937		49.072	1.90	11.31	5
MOTA	1036	CZ3	TRP	142	38.245		43.454		11.65	5
ATOM	1037	CHS		142	38.645		49.089	1.00	9.80	Ē
ATOM ATOM	1038	0	TRP TRP	142 142	43.288 43.380		47.877 49.076	1.00	5.00	6
ATOM	1040	N	LEU	143	44.349		47.109	1.00	6.66	3
ATOM	1041	CA	LEU	143	45.700		47.656	1.00	5.47 3.56	6
ATOM	1042	CB	LEU	143	46.520		47.123	1.00	2.35	é
ATOM	1043	CG	LEU	143	46.031		47.408	1.00	2.00	6
ATOM	1044	CD1	LEU	143	46.832		46.601	1.00	2.00	6
ATOM	1045	CD2	LEU	143	46.182	21.223	48.862	1.00	2.00	5
ATOM	1046	С	LEU	143	46.310		47.158	1.00	2.00	5
MOTA	1047	0	LEU	143	45.765		46.274	1.00	4.81	à
ATOM	1048	N	PRO	144	47.411		47.762	1.00	2.00	7
ATOM	1049	CD	PRO	144	48.003		49.030	1.00	2.00	•
MOTA MOTA	1050 1051	CA CB	PRO PRO	144 144	48.027 48.955		47.295 48.445	1.00	2.00	•
ATOM	1052	CG	PRO	144	48.442		49.601	1.00	2.00 2.00	ş
ATOM	1053	c	PRO	144	48.821		46.011	1.00	2.00	÷
ATOM	1054	C	PRO	144	48.999		45.580	1.00	2.00	į
ATOM	1055	N	PRO	145	49.249	27.823	45.342	1.00	2.00	7
MOTA	1056	CD	PRO	145	49.05	29.249	45.645	1.00	2.00	÷
ATOM	1057	CA	PRO	145	50.022		44.113	1.00	2.72	÷
ATOM	1058	CB	PRO	145	50.53		43.839	1.00	2.80	÷
MOTA MOTA	1059	CG	BBC	145	49.467		44.372	1.00	2.95	Ē
ATOM	1060 1061	0	PRO PRO	145 145	51.176 51.875		44.455	1.00	4.71	•
ATOM	1062	N	PRO	146	51.39		43.639	1.00		<u> </u>
ATOM	1063	CD	PRO	146	50.73		42.347	1.00		÷
ATOM	1064	CA	PRO	146	52.46		43.857	1.00		÷
MOTA	1065	CB	PRO	146	52.35	3 23.778	42.622	1.00		€.
ATOM	1066	CG	PRO	146	50.97		42.167	1.00	5.28	÷
ATOM	10,67	C	PRC	146	53.86		43.967	1.00		÷
ATOM	1068		PRO	146	54.27		43.135		10.56	÷
ATOM	1069	N	GLU	147	54.60		44.975	1.00		7
atom Atom	1070	CA CB	GL"	147	55.95 56.89		45.248 44.077	1.00		÷
ATOM	1072	SG	GLU	147	56.73		43.456	1.00	2.95 18.10	:
ATOM	1073	CD	GLU	147	57.47		44.166		22.76	÷
ATOM	1074		GLU	147	58.33		45.061		25.12	:
ATOM	1075	CE2	GLU	147	57.20		43.789		23.73	:
ATOM	1076	2	GLT	147	56.05		45.624		10.12	÷
MOTA	1077	3	GLU	147	57.09		45.453		12.66	3
MOTA	1075	N	THR	148	54.97		45.124		10.44	:
MOTA MOTA	1079	Ch	THR	148	55.04		46.541	1.00		•
ATOM	1080	CB 2G1	THE THE	148 148	53.77		45.178	1.00		•
ATOM	1082		THR	148	53.58 53.88		44.765 45.621	1.00		•
ATOM	1083	c c	THR	148	55.27		43.048	00		÷ ÷
ATOM	1084	5	THR	146	54.60		43.789	1.00		;
						*				•

bref2	lc.pd	ь		Thu	λpr	25	12	:27	: 47	1996	15	
ATOM	1085	N	PRO	149		56.2		29.		48.503	1.00 7.63	. :
ATOM	1086	CD	PRO	149		57.15		30.4		47.666 49.926	1.00 4.62 1.00 5.20	ŧ
MOTA	1087	CA	PRO	149		56.62 58.0		29.°	-	49.860	1.00 2.62	•
ATOM	1088	CB	PRO PRO	149 149		58.0		31.		48.698	1.00 2.00	•
MOTA MOTA	1089 1090	c	PRO	149		55.7	42	30.		50.498	1.00 7.00	<i>:</i>
ATOM	1091	0	PRO	149		55.0		31.		49.737	1.00 10.83	:
ATOM	1092	N	MET	15σ 150		55.7 54.9		31.	048	52.464	1.00 5.41	÷
ATOM	1093 1094	CA	MET MET	150		55.4			469	52.109	1.00 5.16	ŧ
ATOM ATOM	1095	CG	MET	150		56.8			812	52.512	1.00 2.00	: 15
ATOM	1096	SD	MET	150		57.1			97B 706	54.292 54.546	1.00 8.51 1.00 2.48	- 5
ATOM	1097	CE	MET MET	150 150		57.0 53.4			927	52.169	1.00 5.15	ē,
atom atom	1098 1099	0	MET	150		52.7		32.	952	52.002	1.00 4.08	
MOTA	1100	N	THR	151		52.8			696	52.239	1.00 3.72	
ATOM	1101	CA	THP.	151		51.4			. 405 . 902	51.963 51.799	1.00 2.22	
ATOM	1102 1103		THR THR	151 151		51.5			. 183	52.955	1.00 8.69) ?
MOTA MOTA	1104		THR	151		51.			.347	50.609		_
ATOM	1105	С	THR	151		50.49.			.920 .919	52.922 52.583		
ATOM	1106		THP. SER	151 152		50.			.331	54.123	1.00 6.43	2 7
ATOM ATOM	1107		SER	152		49.	_		. 831	55.04		1 :
ATOM	1109		SER	152		50.			.598	36.47		
MOTA	1110		SER	152		51.	563		.645	56.893 54.843		
ATOM	1111		SER SER	152 152			982		.976	55.68	1.00 10.3	
MOTA MOTA	1112		HIS	153		50.	148	33	.866	53.78		-
ATOM	111			153			070		.291	53.48		
MOTA	1113			153			479 310		. 883 5. 975	53.27 54.52		
ATOM	111		HIS 2 HIS	153 153			810		.048		2 1.00 3.8	4
MOTA MOTA	111		1 HIS			52.	781	34	. 868			
ATOM	111		1 HIS				540		5.254 6.570			_
MOTA	112		2 HIS HIS				. 573 . 275		5.491			4 5
MOTA MOTA	112 112		RIS				.013	3 3	6.614	51.81		
MOTA	112		ILE	154			. 937		4.385			00 7
ATOM	112						. 201 . 493	_	4.412 3.116		_	00 ÷
MOTA			B ILI G2 ILI				. 900		3.208		6 1.00 2.0	
MOTA MOTA			G1 IL			49	. 982		2.883			
ATOM			D1 IL				.30		4.53			
ATOM							.70		3.89			
ATOM ATOM		-		_			.06		5.39	1 49.8		20
ATOM			A AR	G 15			. 63		5.64		· · · · · · · · · · · · · · · · · · ·	20 E
ATOM	111		B AR				1.37 1.59	_	37.14 37.92			42
ATO		-	G AR				1.38	-	39.39			
ATO: ATO:	-		TE AF			4	1.20	16 4	40.10			
ATO:	4 11	37 (Z AF			4	4.83 5.71		41.22 41.84			
ATO			NH1 AF NH2 AF				4.60		41.70		25 1.00 28.	94 :
ATO OTA		-	C AI			4	4.06	67	34.96			.22
ATO	M 11	41		RG 1:			4.80		34.76			. 2 5
ATO		42 '			56 56		2.0		33.92			.24
ATO ATO					56		1.7		32.4	74 43.		.18
ATO		45	CG T		56		2.9		31.6			
ATO			CD1 T		56 56		3.4		31.5			.29
ATO		147 148	CE1 T CD2 T		56		3.7		31.0	_	341 1.00 14	.47
ATC ATC		149	CE2 I	YP. 1	56	4	14.8	95	30.2	BA 47.	646 1.10 14	.32
ATC	i Mc	150	CZ T	YF. 1	56		15.3		30.2			.23
ATC		151			56 56		16.4 10.7		29.5 34.6		365 1.30 7	.25
ATC ATC		152 153			56		10.1		35.2	04 48.	256 1.00 8	1.19
ATC		154	N G	10 1	57		40.2	86	34.5		107 1.00 4	. 99
ATC	DM 1	155			.57		38.9 39.0		35.0 36.2			20 31
ATC ATC		156 157			.57 .57		37.6		36.8		614	:.E~
TA TA		158	CD (ו טוג	157		37.5	577	38.0	30 43		2.35
TA	OM 1	159	OE1		157		37.5		39.1			2.:: 5.::
AT		1160	OE2 (157 157		37.4 38.3		33.9		997 1.20	4.19
		1161 1162			157		36.		33.		102 1.30 1	0.44

bre£2	1c.pc	ъ		Thu	Apr 25	12:27:47	1996	16
ATOM	1163	N	VAL	158	37.022		45.406	1.00 5.40 :
atom atom	1164 1165	CA	VAL	158	36.196		44.842	1.00 6.15 f
ATOM	1166	CB CG1	VAL VAL	158 158	35.459 34.653		45.954 45.391	1.00 3.03 5
ATOM	1167		VAL	158	36.429		46.962	1.00 4.03 £
ATOM	1168	C	VAL	158	35.154	33.186	43.878	1.00 9.07 5
atom atom	1169	e P	VAL	158	34.400		44.208	1.00 10.93
ATOM	1170 1171	r. Ca	ASP ASP	159 159	35.114 34.147		42.681	1.00 10.57
ATOM	1172	CB	ASP	159	34.828		41.672 40.327	1.00 10.09 5 1.00 11.17 5
ATOM	1173	CG	ASP	159	33.873		39.256	1.00 13.89 6
ATOM	1174		ASP	159	33.863		38.172	1.00 13.65
ATOM ATOM	1175 1176	C C	ASP ASP	159 159	33.093 32.997		39.547	1.00 15.65
ATOM	1177	ō	ASP	159	33.227		41.575	1.00 9.91 5 1.00 11.09 8
ATOM	1178	N	VAL	160	31.766		41.637	1.00 7.83 7
MOTA	1179	CA	VAL	160	30.582		41.535	1.00 5.49 5
ATOM ATOM	1180 1181	CB	VAL VAL	160 160	29.637		42.755	1.00 3.19 4
ATOM	1182		VAL	160	28.512 30.362		42.742 44.091	1.00 3.00 5 1.00 2.00 5
ATOM	1183	c	VAL	160	29.842		40.286	1.00 6.19 5
ATOM	1184	0	VAL	160	29.364		40.238	1.00 8.22 =
atom atom	1185	N	SER	161	29.835		39.300	1.00 7.72 7
ATOM	1186 1187	CA CB	SEP. SER	161 161	29.104 30.094		38.046 36.891	1.00 8.29 5
ATOM	1188	OG	SER	161	30.637		26.934	1.00 10.26 £
ATOM	1189	2	SER	161	28.161		27.938	1.00 7.24 €
atom atom	1190 1191	0	SER	161	28.601		28.024	
ATOM	1192	N CA	ALA ALA	162 162	26.885 25.793		37.791 27.784	1.00 7.94 E 1.00 9.16 7 1.00 12.39 E
ATOM	1193	CB	ALA	162	24.689		38.736	1.00 12.39 ÷
ATOM	1194	С	ALA	162	25.199		36.379	1.00 14.12
ATOM	1195	0	ALA	162	25.593		35.406	1.00 13.91
ATOM ATOM	1196 1197	N CA	GLY	163 163	24.220 23.598		36.369	1.00 15.85 7
ATOM	1198	c	GLY	163	22.561		35.150 34.370	1.00 16.65 5 1.00 18.26 5
ATOM	1199	0	GLY	163	21.996		34.897	1.00 18.80 3
ATOM	1200	N	ASN	164	22.416		33.146	1.00 90.00 7
atom atom	1201 1202	CA CB	asn asn	164 164	21.568 20.505		21.994	1.00 90.00 5
ATOM	1203	CG	ASN	164	19.337		31.685 32.702	1.00 90.00 £
MOTA	1204		ASN	164	19.322		33.726	1.00 90.00 =
ATOM	1205		ASN	164	18.334		32.511	1.00 90.00 7
atom atom	1206 1207	5	asn asn	164 164	20.728 19.665		22.186	1.00 90.00 5
ATOM	1208	N	GLY	165	21.227		32.817 31.601	1.00 90.00 3 1.00 90.00 7
MOTA	1209	CA	GLY	165	20.544		31.514	1.00 90.00 5
ATOM	1210	ç	GLY	165	20.274		32.859	1.00 90.00 ÷
atom atom	1211 1212	C N	GLY ALA	165 166	19.470 20.941		32.927	1.00 90.00 5
ATOM	1213	CA	ALA	166	20.541		33.967 35.242	1.00 90.00 - 1.00 90.00 -
ATOM	1214	CB	ALA	166	19.550		35.015	1.00 90.00 4
ATOM	1215	C	ALA	166	21.795		36.188	1.00 90.00 5
ATOM ATOM	1216 1217	O N	ALA GLY	166 167	21.646 22.964		37.421	1.00 90.00 3
ATOM	1218	CA	GLY	167	24.167		35.614 36.400	1.00 11.62 7 1.00 13.44 5
ATOM	1219	C	GLY	157	24.110		35.704	1.00 15.68
ATOM	1220		GLY	167	23.701		25.863	1.00 15.58 3
ATOM ATOM	1221 1222	N CA	SER SER	168 168	24.504 24.434		37.909	1.00 17.86
ATOM	1223	CB	SER	168	23.543		38.252 39.465	1.00 18.83
ATOM	1224	OG	SER	168	22.558		39.118	1.00 23.47
MOTA	1225	Ċ	SER	168	25.820		38.537	1.60 18.61
ATOM ATOM	1226 1227	() ()	SER Val	16R 169	25.961 26.808		38.506	1.00 18.81 =
ATOM	1228	CA	VAL	159	28.218		28.789 39.149	1.00 18.64 1.00 17.78
ATOM	1229	CB	VAL	169	28.719	39.141	38.657	1.00 19.01
ATOM	1230		VAL	169	30.262		38.769	1.00 16.57
MOTA MOTA	1231 1232	CGS	VAL	169 169	28.407 28.387		37.197	1.00 18.24
ATOM	1233	õ	VAL	169	28.222		40.666	1.90 17.25 ÷
ATOM	1234	N	GLN	170	28.725		41.201	1.00 15.44
ATOM	1235	CA	GLN	170	28.905		42.647	1.00 17.12
ATOM ATOM	1236 1237	CB	GLN GLN	170 170	27.928 27.921		43.231	1.00 19.39
ATOM	1238	CD	GLN	170	28.202		44.766 45.365	1.00 24.35 4 1.00 26.34 4
ATOM	1239	OE1	GLN	170	27.369		45.247	1.00 27.24 4
ATOM	1240	NE.2	GLN	170	29.33	5 33.868	46.004	1.00 28.12

bre£21	.c.pdl	5		Thu	Apı	25	12:	27:47	199	96		17	
ATOM	1241	С	GLN	170		30.34		6.030	43.0		.00 14		ė.
ATOM	1242	0	GLN	170		30.73		4.892	42.8		.00 10		5 7
ATOM	1243	N	ARG	171		31.10		6.932	43.6		.00 13		•
MOTA	1244	CA	ARG	171		32.47		7.718	43.5		.00 13		6
MOTA	1245	CB CG	ARG	171 171		33.54		7.814	42.0		.00 12		5
ATOM ATOM	1245	CD	ARG	171		34.46		6.758	41.4		.00 13		5
ATOM	1248	NE	ARG	171		34.62		6.922	39.		.00 10		7 5
ATOM	1249	CZ	ARG	171		25.27		7.932	39.3 40.3			.84 .37	7
MOTA	1250		ARG	171		35.84 35.30		8.000	38.			. 87	7
ATOM	1251 1252	NH2 C	ARG	171		32.58		6.543	45.		.00 15		5
atom atom	1253	ŏ	ARG	171		31.70		37.062	46.		1.00 17		3
ATOM	1254	N	VAL	172		33.6		35.916	46.	1 1	1.00 11		7 5
ATOM	1255	CA	VAL	172		33.8		35.727			1.00 9	1.19	6
ATOM	1256	CB	VAL	172		33.4		34.260 34.155				5.41	5
ATOM	1257		VAL	172 172		32.2		33.745	_		1.00 1		6
ATOM	1258 1259	C	VAL	172		35.2		35.966	48.			9.92	6
ATOM ATOM	1260	ŏ	VAL	172		36.1		35.398			1.00 1		3
ATOM	1261	N	GLU	173		35.3		36.778			1.00 1		7 5
MOTA	1262	CA	GLU	173		36.6		37.041 38.463		657 218	1.00 1		6
ATOM	1263	CB	GLU	173		36.7 36.5		39.569		173	1.00 2		5
MOTA	1264	CC	CTO CTO	173 173		37.2		40.903		573	1.00 2		5
ATOM	1265 1266	CD	CLU			37.7		41.647		649	1.00 2	3.21	3
atom atom	1267		2 GLU			37.3		41.206		. 803	1.00 2		3
ATOM	1268	c	GLU			26.9		36.016	-	.779	1.00 1		
ATOM	1269	٥	GLU			36.0		35.720		.592	1.00 1		3 7
ATOM	1270	N	ILE			38.0		35.403 34.400		.719 .669	1.00 1		6
MOTA	1271	CA	ILE			38.5		33.089		. 966	1.00		6
MOTA	1272	CB				40.0		32.38		. 689	1.00		5
MOTA MOTA	1273 1274		1 ILE			37.		32.18	2 50	.893	1.00		6
ATOM	1275		1 ILE			36.	625	32.62		. 917	1.00		6
ATOM	1276	_	ILI	17	4	39.		35.05		.250	1.00		6 9
ATOM	1277	0	IL			40.		35.69	·	.532	1.00		7
ATOM	1278		LE			39.		34.95 35.58		.558	1.00		6
ATOM	1279					41.	838	35.97		. 609	1.00		6
ATOM	1280						467	37.46		. 733	1.00		6
ATOM	1281 1282		1 LE	_			100	38.11		1.394	1.00	14.03	6
MOTA MOTA	1283		2 LE				345	37.62		5.733	1.00		5
ATOM	1284		LE		5		394	34.75		1.031	1.00		5 8
ATOM	128	0	LE				322	33.53		3.838 4.084	1.00	17.18	ž
ATOM	128		GL				542 842	35.43 34.76	-	3.946		16.66	5
ATOM	128						000	35.73		4.145		21.33	5
atom Atom	128 128			_			963	36.47		5.432		20.62	5
ATOM	129	-				46.	145	37.92	_	5.180		22.84	5
ATOM	129		El Gl		76		.330	38.34		5.218		23.62	9 8
ATOM	129	2 0	E2 GI		16		.117	38.6		4.911 4.852		23.22 12.93	į
ATOM	129				76		.068 .875	33.6		5.062		16.37	•
MOTA	129				76 77		.574	32.5		4.259	1.00	9.95	
MOTA	129 129		A GI		 לכ		. 839			5.001	1.00	8.11	
atom Atom					רר		.738	20.3	40 5	4.827		7.43	
ATOM					77		. 990			4.962		9.00	
ATOM					78		.534			4.493		7.50 8.26	
ATOM					78		.398			54.316 54.477		10.81	
ATOM	. •				78		.116			5.616		14.76	5 5
ATOM					78 .78		911	_		56.950		20.12	? :
10tk 10tk					78		. 904			57.960	1.00	24.00	7
ATC					78		.400	32.5	509	58.13		26.2	
ATO			NH1 A	RG 1	78		2.004			57.38		27.3	2 7
ATC		07	NH2 A	RG 1	178		3.35			59.04		26.5	
ATO					178		2.37: 2.48			52.95¢ 51.93¢			
ATO					178 179		2.20			52.93			7 7
DTA DTA					179		2.14			51.68			1 ÷
ATO					179		3.37	6 26.	310	51.54	2 1.0		2 5
אדס			OG1 1	rhr.	179		3.65			52.81		12.7	
ATO	M 13	14	CG2 1	rhr	179		4.55			51.07		0 6.0 0 14.1	
ATO		15			179		0.87		265 102	51.64 51.15		0 14.1 0 15.4	
ATO		16			179 180		0.89 9.77		831	52.15		0 13.3	
ATO ATC		117		GLU GLU	180		E. 46		188	52.16		0 12.9	
W1.C						•							

bref2	lc.pd	Ь		Thu	Apr 25 12	:27:47	1996	18
ATOM	1319	СВ	GLU	180	38.329	25.242	53.340	1.00 14.42 5
ATOM	1320	CG	GLU	180		24.052	53.048	1.00 18.37 6
ATOM	1321	CD	GLU	180		23.255	54.299	1.00 19.86 6
ATOM	1322	0E1		180	36.526	23.877	55.216	1.00 21.31
ATOM	1323	OE2		180	37.473	22.045	54.387	1.00 18.58 8
ATOM	1324	C	GLU	180	37.442	27.288	52.301	1.00 14.56
ATOM	1325	0	GLU	180	37.742	28.385	52.782 51.934	1.00 14.76 & 1.00 13.82 7
ATOM ATOM	1326 1327	N CA	CYS	181 181	36.209 35.149	26.986 27.967	52.034	1.00 13.82 7 1.00 12.64 5
ATOM	1328	CB	CYS	181	35.382	28.990	50.936	1.00 12.66 5
ATOM	1329	SG	CYS	181	33.911	29.643	50.288	1.00 13.38 15
ATOM	1330	c	CYS	181	33.766	27.287	51.905	1.00 13.84 6
ATOM	1331	0	CYS	181	33.606	26.383	51.086	1.00 15.56 8
ATOM	1332	N	VAL	182	32.790	27.639	52.743	1.00 13.12 7
MOTA	1333	CA	VAL	182	31.478	26.985	22.613	1.00 11.97 6
ATOM	1334	CB	VAL	182	31.093	26.072	53.820	1.00 9.54 6
ATOM	1335		VAL	182	32.003	26.307	55.003	1.00 10.81 6
ATOM ATOM	1336 1337	C	VAL VAL	182 182	29.669 30.353	26.255 27.910	54.193 52.171	1.00 8.15 6 1.00 12.84 6
ATOM	1338	0	VAL	182	29.930	28.828	52.872	1.00 13.90 3
ATOM	1339	N	LEU	183	29.954	27.715	50.930	1.00 11.79 7
ATOM	1340	CA	LEU	183	28.921	28.515	50.338	1.00 12.76 5
ATOM	1341	CB	LEU	183	29.052	28.500	48.817	1.00 13.26 6
ATOM	1342	CG	LEU	183	30.193	29.380	43.350	1.00 11.81 6
ATOM	1343	CD1	LEU	183	30.636	28.956	46.970	1.00 8.24 6
ATOM	1344		LEU	183	29.734	30.852	43.398	1.00 13.01 5
MOTA	1345	C	LEU	183	27.564	28.027	53.778	1.00 14.24 5
ATOM	1346	0	LEU	183	27.139	26.887	53.514	1.00 15.09 3
ATOM	1347	N	SER	184	26.897	28.909	51.487	1.00 14.69 7
ATOM	1348	CA	SER	184	25.583	28.642	11.998	1.00 16.60 6
ATOM	1349	CB OG	SER	184	25.558	29.046	53.461	1.00 17.40 6
atom atom	1350 1351	C	ser Ser	184 184	26.601 24.671	28.369 29.537	54.144 51.208	1.00 18.79 à 1.00 17.61 6
ATOM	1352	ō	SER	184	25.115	30.545	50.679	1.00 18.84 3
ATOM	1353	N	ASN	185	23.422	29.140	51.048	1.00 18.50 7
ATOM	1354	CA	ASN	185	22.479	29.998	50.338	1.00 21.04 6
ATOM	1355	CB	ASN	185	22.463	31.389	51.008	1.00 27.82 6
ATOM	1356	CG	ASN	185	22.274	31.330	52.546	1.00 33.52 6
ATOM	1357		ASN	185	22.899	32.131	53.270	1.00 36.61 8
ATOM	1358		ASN	185	21.392	30.414	53.050	1.00 36.25 7
ATOM	1359	C	ASN	185	22.641	30.149	49.794	1.00 19.48 6
MOTA MOTA	1360 1361	0	asn Leu	185 186	22.967 22.329	31.228 29.062	43.263 43.093	1.00 18.46 à 1.00 17.53 7
ATOM	1362	CA	LEU	186	22.384	28.972	46.635	1.00 15.82
ATOM	1363	CB	LEU	186	23.632	28.170	46.201	1.00 14.99 6
ATOM	1364	CG	LEU	196	25.006	28.318	45.924	1.00 15.24 5
ATOM	1365	CD1	LEU	186	25.951	27.172	45.540	1.00 13.51 5
ATOM	1366	CD2	LEU	136	25.689	29.663	46.637	1.00 14.02 6
ATOM	1367	ε	LEU	196	21.069	28.230	45.261	1.00 16.15
ATOM	1368	0	LEU	186	20.449	27.566	47.116	1.00 16.6B a
ATOM	1369	N	ARG	187	20.611	28.382	45.019	1.00 15.66 7
MOTA	1370	CA	ARG	187 187	19.371 18.845	27.749	44.576	1.00 14.27 6
MOTA MOTA	1371 1372	CB	ARG ARG	187	19.153	28,415 29.870	43.263	1.00 14.63 6 1.00 19.73 5
ATOM	1373	CD	ARG	187	18.525	30.512	42.054	1.00 23.74 5
ATOM	1374	NE	ARG	187	19.218	30.197	40.905	1.00 25.90 7
ATOM	1375	CZ	ARG	187	18.997	29.109	43.060	1.00 29.07 5
ATOM	1376		ARG	187	18.110	28.181	40.430	1.00 29.72 7
ATOM	1377	NH 2	ARG	187	19.594	29.001	33.874	1.00 31.36 7
MOTA	1378	¢	ARG	187	19.528	26.264	44.298	1.00 16.07 5
ATOM	1379	9	ARG	187	20.608	25.788	43.872	1.00 14.20
ATOM	1380	N	GLY	138	18.413	25.55? 24.124	44.483	1.00 15.94 T
atom atom	1381 1382	CA C	GLY	188 188	18.369 18.304	23.695	42.842	1.00 17.35 & 1.00 19.74 6
ATOM	1382	ě	GLY	188	17.760	24.421	42.016	1.00 20.69
ATOM	1384	N	ARG	189	18.823	22.492	42.563	1.00 20.12 7
ATOM	1385	CA	ARG	129	18.891	21.885	41.239	1.00 20.15 #
ATOM	1386	CB	ARG	169	17.495	21.501	41.731	1.00 20.15 # 1.00 22.54 f
ATOM	1387	CG	ARG	189	17,450	20.203	33.971	1.00 25.04 6
ATOM	1388	CD	AP.G	159	17,780	20.447	38.38C	1.00 25.92
ATOM	1389	NE	AP.G	169	18.570	19.373	37.756	1.00 27.40 7
MOTA	1390	CZ	ARG	189	18.076	18.215	37.299	1.00 29.60 8
MOTA	1391		1 AF.G	189	16.768	17.937	37.405	1.00 39.45
ATOM	1392		2 ARG	129	18.886	17.342	35.686	00 29.39 7
MOTA MOTA	1393 1394	S	ARG	189	19.610	22.773	43.218	1.00 20.12 ÷
MOTA	1394	Ŋ	ARG THR	199 190	19.40€ 20.432	22.605 23.719		
ATOM	1396			190	21.195	24.611		

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ATOM	1397	СВ	THR	190		21.494	25.944	40.460	1.00 15		
MOTA	1398	0G1	THP.	190		20.370	26.366	41.226	1.00 18		
MOTA	1399		THR	190		21.869 22.576	26.984	39.612	1.00 17		
ATOM	1400	c	THR	190 190		23.024	23.222	40.428	1.00 17	.12	
ATOM	1401 1402	0 N	ARG	191		23.262	24.460	28.563	1.00 18		
ATOM ATOM	1403	CA	ARG	191		24.621	24.01B	38.253	1.00 18		: £
ATOM	1404	CB	ARG	191		24.783	23.686	35.746 35.278	1.00 23		•
MOTA	1405	CG	ARG	191		26.243 26.802	23.477 22.032	35.502	1.00 29		
ATOM	1406	CD	ARG	191 191		26.824	21.206	25.274	1.00 31	.41	7
MOTA MOTA	1407	NE CZ	ARG	191		27.677	21.329	34.236	1.00 30		•
ATOM	1409		ARG	191		28.650	22.261	24.198	1.00 30		7
ATOM	1410	NH2	ARG	191		27.562	20.481	33.210	1.00 30		į
MOTA	1411	C	ARG	191		25.471	25.213	38.627 28.233			5
ATOM	1412	0	ARG	191 192		25.174 26.495	26.344 24.950	39.417			7
MOTA	1413	N CA	TYR TYR			27.380	25.971	39.901		1.03	÷
MOTA MOTA	1415	CB	TYP			27.283	26.027	41.411			é
ATOM	1416	CG	TYR	192		26.063	26.759				6 6
MOTA	1417		TYR			26.105	28.138				÷
MOTA	1418		TYP			24.949 24.837	28.867				÷
MOTA	1419		YYF YYF			23.670	26.840			5.93	ş.,
ATOM ATOM	1421	CZ.	TYF			23.745	28.217				ř
ATOM	1422	OH	TYF			22.618	28.972				± 4
MOTA	1423		TY			28.759	25.557 24.402				
ATOM	1424		TYI			29.134 29.511	26.491				ē -
MOTA	1425 1426		THI THI	_		30.875				7.07	ŧ.
MOTA MOTA	1427					31.036		27.02		7.66	÷
ATOM	1428		1 TH	_		30.030				5.74 7.11	3 6
MOTA	1429		2 TH			32.399				7.05	5
ATOM	1430		TH			31.688 31.370				7.20	3
MOTA	1431		TH Ph			32.685				8.39	7
MOTA MOTA	1432			_		33.487				5.90	5
ATOM	1434	_			4	33.421				6.97	ŕ
ATOM	143	5 C			94	32.030				8.68 5.87	é
atom	143		01 PH		94	31.533 31.223				8.15	÷
MOTA	143		02 PH E1 PH		94 94	30.27				8.14	5
ATOM ATOM	143		E2 PF		94	29.95		2 43.94		5.23	5
ATOM	144				94	29.48		9 43.7		7.24 5.55	é
MOTA	144		Pi		94	34.92				6.55	
MOTA	144				94 95	35.36 35.64				5.34	3
MOTA MOTA	144 144				95	37.05				4.57	•
ATOM	144				95	37.17				5.31	÷
ATOM	144				95	37.74				3.32 2.79	÷
ATOM	144				95	37.10 39.03	_			2.76	ŕ
ATOM	144				.96 .96	39.83				3.78	÷
MOTA MOTA					96	40.52			69 1.00		÷
ATOM			G1 V		96	40.23	30.2				ě
ATOM	14:	52 (:G2 V		196	40.13					•
ATOM					196	41.00					3
ATOM		54 . (196 197	41.5					7
ATOM ATOM					197	42.6	87 32.8				÷
ATON					197	42.2					•
ATON	1 14				19?	41.3					÷
ATON					197	41.0 40.3					÷
ATO				ARG ARG	197 197	40.2		-			•
ATO: ATO:			NH1		197	40.8		550 39.	357 1.00	2.00	:
ATO			NH2	ARG	197	39.7					
ATO	M 14	64	C .	ARG	197	43.3			362 1.00 280 1.00		
ATO		65		ARG	197	42.€ 44.7			399 1.0		
ATO ATO		166 167		ALA ALA	198 198	45.4			550 1.0	C 2.47	•
OTA OTA		168		ALA	198	46.4	20 32.	903 45.	072 1.0	0 2.30) :
ATO		169	Ċ.	ALA	198	46.2			442 1.0		
ATO	M 1	470	0	ALA	198	46.			.340 1.0 .612 1.0		
ATC		471	N	ARG ARG	199 199	46.: 47			694 1.0		
ATC ATC		472 473	CA CF	ARG	199	46.			.572 1.0		
ATO		474	CG	ARG	199				.270 1.0	00 5.6	7

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ATOM	1475	CD	ARG	199	45.9	38	40.737	45.915	1.00	9.17	5
ATOM	1476	NE	ARG	199	46.3		42.120	45.579	1.00	13.78	=
ATOM	1477	CZ	ARG	199	46.1		42.662	44.363		15.94	٤
atom atom	1478 1479	NH1 NH2		199 199	45.7 46.4		41.950	43.339		18.32	:
ATOM	1480	C	ARG	:99	48.0		43.954 37.321	44.181	1.00	18.45	5
ATOM	1481	õ	ARG	199	47.5		36.916	48.058	1.00	8.08	:
ATOM	1482	N	MET	200	49.2	243	37.864	46.984	1.00	5.53	:
ATOM	1483	CA	MET	200	50.0		38.096	48.197	1.00	4.85	÷
ATOM	1484	CB	MET	200	51.4		38.423	47.891	1.00	3.73	5
ATOM ATOM	1485 1486	CG SD	MET MET	200 200	52.3 53.2		37.271 36.286	47.346 48.538	1.00	4.67	ნ 15
ATOM	1487	CE	MET	200	52.2		34.975	48.812	1.00	9.73 2.41	5
ATOM	1488	С	MET	230	49.3		39.289	48.874	1.00	7.02	ė
ATOM	1489	0	MET	200	49.0		40.314	48.228	1.00	6.42	3
ATOM	1490	N CA	ALA	201	49.0		39.126	50.167	1.00	7.96	:
ATOM ATOM	1491 1492	CB	ALA ALA	201 201	48.3 47.6		40.140 39.474	50.962 52.117	1.00	10.65	5 5
ATOM	1493	c	ALA	201	49.2		41.285	51.464		4.85 12.36	5
ATOM	1494	0	ALA	201	50.4		41.204	51.453		13.02	3
ATOM	1495	N	GLU	202	48.6		42.360	51.901		15.72	7
MOTA	1496	CA	GLU	202	49.3	336	43.527	52.421		19.04	5
ATOM	1497	CB	GLU	202	48.4		44.756	52.276		23.13	s,
MOTA	1498	CG	GLU	202	47.6		44.796	50.914		28.94	5
ATOM ATOM	1499 1500	CD O£1	GLU GLU	202 202	48.3 49.4		45.575 46.164	49.757 49.968		31.22	:
ATOM	1501	OE2	GLU	202	47.7		45.613	48.634		32.80	1
MOTA	1502	c	GLU	202	49.7		43.317	53.903		19.11	÷
ATOM	1503	0	GLU	202	49.3		42.327	54.561		20.41	3
ATOM	1504	N	PRO	293	50.6		44.173	54.411		16.25	7
ATOM ATOM	1505 1506	CD	PRO	203	51.1		44.143	55.820		15.32	5
ATOM	1507	CA CB	PRO PRO	203 203	51.3 51.3		45.290 46.367	53.714 54.782		14.26	6
ATOM	1508	CG	PRO	203	51.6		45.538	55.984		16.38	6 5
ATOM	1509	Ç	PRO	203	52.7		44.892	53.356		12.03	6
ATOM	1510	0	PRO	203	53.5	537	45.743	52.985		15.28	3
ATOM	1511	N	SEP.	204	53.0		43.623	53.540	1.00	8.98	7
ATOM	1512	CA	SEP.	204	54.4		43.146	53.222		11.79	5
ATOM ATOM	1513 1514	CB OG	SEP. SEP.	204 204	54.6 55.0		41.764	53.868		11.87	5
ATOM	1515	C	SER	204	54.6		43.060	55.224 51.696		12.48	•
ATOM	1516	ō	SER	204	55.6		43.660	51.152		11.24	į
ATOM	1517	N	PHE	205	53.6	918	42.309	51.031		10.89	7
MOTA	1518	CA	PHE	205	53.9		42.074	49.624	1.00	8.76	÷
MOTA	1519	CB	PHE	205	53.9		40.573	49.390	1.00	8.70	5
ATOM ATOM	1520 1521	CG	PHE PHE	205 205	55.0 54.1		39.862 38.885	50.052 51.029		12.81	÷
ATOM	1522		PHE	205	56.		40.136	49.668		11.00	
ATOM	1523		PHE	235	55.9		38.198	51.599	1.00	7.35	÷
ATOM	1524		PHE	205	57.4		39.449	50.237		11.11	÷
ATOM	1525	CZ	PHE	205	57.		38.480	51.202	1.00	8.98	:
ATOM ATOM	1526 1527	o o	PHE	205 205	52. 51.		42.728 43.147	48.900 49.508	1.00	8.87	÷
ATOM	1528	Ŋ	GLY	206	52.	913	42.864	47.592	1.00	9.29 8.57	= =
ATOM	1529	CA	GLY	206	51.		43.459	46.751	1.00	8.14	÷
ATOM	1530	С	GLY	206	52.		42.855	45.367	1.00	7.24	-
ATOM	1531	9	GLY	206	52.		42.124	45.081	1.00	8.58	***************************************
ATOM	1532		GLY	207	51.		43.080	44.520	1.00	7.18	:
atom Atom	1533 1534	CY C	GLY	207 207	51. 49.		42.534 42.355	43.176	1.00	7.59	•
ATOM	1535	õ	GLY	207		857	43.048	42.430 42.656	1.00	4.80 5.05	7
ATOM	1536	N	PHE	228	49.		41.332	41.608	1.00	3.71	
MOTA	1537	CA	PHE	208	48.	621	41.069	40.805	1.00	3.73	÷
ATOM	1536	CB	PHE	208		034	41.071	39.322	1.00	6.46	de de en de de de en de
ATOM	1539	SG	PHE	228		158	42.013	39.011	1.00	6.53	:
ATOM ATOM	1540 1541		PHE	208 208		956 441	43.377	39.004 38.793	1.00		•
ATOM	1542		PHE	208		022	44.253	28.790	1.00		:
ATOM	1543		PHE	208		506	42.393	38.579	1.00		
ATOM	1544	CZ	PHE	208	52.	292	43.756	38.580	1.00	6.95	•
ATOM	1545	C	PHE	208		896	39.767	41.149	1.00		÷
atom atom	1546 1547	N	PHE	208		463	38.823 39.780	41.704	1.00		
ATOM	1548	CA.	TP.P TP.P	209 209		766	38.625	40.878 41.073	1.00		:
ATOM	1549	CB	TPP	209		302	38.979	40.811	1.00		
MOTA	1550	CG	TRP	209	43.	505	39.378	42.011	1.00		:
ATOM	1551		TP.P	209		15€	38.550	43.104	1.00	2.67	3
atom	1552	CE	TP.P	209	42.	347	39.316	43.959	1.00	2.87	:

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ATOM	1553	CE3	TRP	209	43.4		7.234	43.446	1.00 2.00	
ATOM	1554	CD1		209	42.9		0.586	42.240	1.00 2.25 6 1.00 2.00 7	
ATOM	1555	NE1	TRP	209	42.2		0.554 6.809	43.396 45.148	1.00 2.00 1 1.00 4.70 5	
MOTA	1556	CZ2		209 209	41.8 42.9		6.729	44.616	1.00 4.57 5	
ATOM	1557 1558	C23 CH2		209	42.1	_	7.513	45.461	1.00 4.76	
MOTA MOTA	1559	c	TRP	209	46.2	22 3	7.604	49.033	1.00 3.17 5	
ATOM	1560	٥	TRP	209	46.5		7.969	33.920	1.00 3.26	
ATOM	1561	N	SER	210	46.2		6.335 5.269	40.412	1.00 4.99	
MOTA	1562	CA	SER	210	46.6 46.9		4.002	40.327	1.00 4.60	
MOTA	1563 1564	CB OG	SER SER	210 210	45.		3.363	40.660	1.00 3.40 3	
atom atom	1565	c	SER	210	45.		4.968	38.515	1.00 9.36	
MOTA	1566	č	SER	210	44.		5.689	18.398	1.00 13.86	
ATOM	1567	N	ALA	211	45.		23.924	37.735 36.757		, 5
ATOM	1568	CA	ALA	211	44. 45.		33.423 32.571	35.768		ò
MOTA	1569 1570	CB C	ala Ala	211 211	43.		32.558	27.567	1.00 11.25	ń
atom atom	1571	Ö	ALA	211		160	32.175	38.706		ē
ATOM	1572		TPP	212			32.263	37.014		7 5
MOTA	1573		TRP	212			31.433	27.734 26.993		÷
MOTA	1574		TRP	212			31.434 32.765	35.942		÷
MOTA	1575		TP.P TRP	212 212			33.399	33.030	1.00 2.00	÷
ATOM	1576 1577		TRP	212			34.597	37.547		÷
ATOM ATOM	1578		TRP	212	38.		33.063	23.3€7	1.00 2.00	÷
MOTA	1579	CD:	TRP	212			33.576	35.867	1.00 2.00	5
MOTA	1580		TPP	212			34.680 35.470	26.219 33.359	1.00 2.00 1.00 4.55	5
MOTA	1581		TRP	212 212		.811 .162	33.921	43.167		6
MOTA MOTA	1582 1583		3 TRP 2 TRP	212		. 640	35.111	39.671	1.00 2.13	ż
MOTA	158		TRP	212		.340	30.012			5
MOTA	158		TRP	212		. 262	29.696			3
MOTA	158		SET	213		.771	29.145			5
MOTA	158			213 213		.222 .041	27.183			ş
ATOM	158	_		213		.667	27.131			ક
ATOM ATOM	158 159	-	SER	213		.303	26.959	37.738		5
MOTA	159		SER	213		.265	27.471			3
MOTA	159	2 N	GLU	214		. 644	25.718			5
ATOM	159			214		.694	24.971			5
ATOM	159 159			214 214		.107	23.79	_	3 1.00 23.12	÷
MOTA MOTA				214	41	.249	24.29			•
ATOM		7 03	1 GLU	214		. 627	25.33			3
MOTA			2 GLU	214		0.218 9.550	23.63			÷
ATOM			GLU	214 214		9.793	24.62			÷
ATOM ATOM			GLU PRO	215		8.301	25.03			
ATOM				215		7.959	25.36			÷
ATCM				215		7.068	24.96			5
ATOM	160			215	_	6.155	25.89			5
ATOM						6.430 6.378	25.44 23.60			ક
ATO: ATO:						6.664	22.65		5 1.00 12.44	ŧ
ATO					. 3	5.440				:
ATC	4 16	09 C	a val		_	4.669				÷
ATO		10 . 0	B VAL		_	4.740				é
ATO			G1 VAI G2 VAI		_	5.226				é
ATO ATO	_		WAI		_	3.261	22.83	34 39.2	59 1.20 9.31	ē
ATC	_		VA		•	3.001			45 1.30 10.20	•
ATC	_		i SEI			2.357				
ATC			CA SEI			26.952				,
ATO			3 SE			20.549 29.610				:
ATC			OG SE!			30.127			C1 30 10.91	:
OTA STA			3 3E		-	30.424	20.0	81 39.6	47 30 9.60	:
ATC			N LE	r 21	8	29.06				
ATO	M: 1	522	CA LE			28.223				
ATC			CB LE		-	28.60 27.99				
ATO			CG LE CD1 LE			28.20				
ATO ATO			CD2 LE		•	28.64			5350 8.78	
ATC		627	S LE			26.72	7 21.2	08 43.		
AT		628	o LE	.U 21	. В	26.30				
AT	CM 1	629	N LE			25.95				
AT	OM 1	630	CA LE	.U 21	. 9	24.48	£ 20.	.04 47.	1.00 13.32	

bref2	lc.pd	Ъ		Thu	Apr 25 1	2:27:47	1996		22	
ATOM	1631	CB	LEU	219	23.867	18.372	40.209	1.00	13.95	÷
ATOM	1632	CG	LEU	219	23.819	18.429	23.736		16.57	5
ATOM	1633	CD1	LEU	219	22.857	19.303	37.947		18.05	5
MOTA	1634	CD2		219	25.208	18.413	23.096		15.67	:
atom atom	1635 1636	0	LEU	219	24.080	20.226	42.248		12.96	÷
ATOM	1637	Ñ	THP.	219 220	24.37E 23.501	19.295 21.339	42.986 42.692		12.64	7
ATOM	1638	CA	THP.	220	23.057	21.472	44.068		12.52 10.27	÷
ATOM	1639	CB	THP.	220	22.289	22.744	44.250		10.53	ē.
MOTA	1640	OG1	TEP	220	22.030	23.330	42.967		14.44	į
MOTA	1641	CG2	THP	220	23.076	23.704	45.099		13.55	:
MOTA	1642	С	THR	220	22.111	20.325	44.368	1.00	11.61	÷
MOTA	1643	0	THP	220	21.196	20.053	43.582	1.00	13.03	=
ATOM	1644	N	THP.	303	67.975	42.354	64.372		11.41	7
ATOM ATOM	1645 1646	C3	THP.	303 303	67.750	41.604	65.597	1.00	9.49	£
ATOM	1647	0G1	THE.	303	66.400 65.988	42.008 43.329	66.344 65.963		10.05	÷
ATOM	1648	CG2	THF.	303	66.595	42.033	67.861		12.85 12.80	5
ATOM	1649	c	THR	303	67.737	40.103	65.280	1.00	9.93	÷
ATOM	1650	٥	THP.	303	68.525	39.342	65.838	1.00	9.37	į
MOTA	1651	N	TYP	304	66.882	39.690	64.343		10.17	7
ATOM	1652	CA	TYP.	304	66.756	38.281	63.973	1.00	9.53	5
ATOM ATOM	1653	C3	TYF.	304	65.306	27.326	64.148	1.00	7.06	5
ATOM	1654 1655	CG CD1	TYP. TYP.	304 304	64.839 64.311	37.927	65.585	1.00	7.97	•
ATOM	1656	CEI	TYF.	304	€4.003	39.123 39.268	66.072 67.389	1.00	4.80	•
ATOM	1657	CD2	TYF.	304	65.030	36.880	66.486	1.00	3.80 6.93	÷
MOTA	1658	CE2	TYF.	394	64.721	37.215	67.809	1.00	4.43	4
MOTA	1659	CZ	TYP.	304	64.208	38.211	68.261	00	4.88	÷
MOTA	1660	CH.	TYF.	304	63.886	38.359	69.598		10.24	÷
MOTA	1661	C	TYP	304	67.182	38.065	62.554	1.00	8.23	÷
MOTA	1662	0	TYP.	304	67.277	39.024	61.804		11.69	3
MOTA MOTA	1663 1664	N CA	SEP. SEP.	305 305	67.474	36.819	62.201	1.00	8.34	7
ATOM	1665	CB	SEF.	305 305	67.856 69.204	36.442 35.705	60.843 60.838	1.00	9.43 13.12	6 5
ATOM	1666	ōG	SEP.	305	70.226	36.516	61.427		18.03	8
ATOM	1667	ε	SEP.	305	66.736	35.557	60.273		10.05	6
ATOM	1668	0	SER	305	66.490	34.433	60.754		10.34	â
ATOM	1669	N	CYS	306	66.093	36.051	59.218	1.00	8.05	7
ATOM	1670	CA	CXE	306	64.968	35.364	58.619	1.00	5.52	ó
ATOM	1671	č	CX	306	64.970	35.039	57.131	1.00	6.70	ě
MOTA MOTA	1672 1673	C 3	CXE	306 306	65.609	35.702	56.302	1.00	6.69	:
ATOM	1674	3G	CYS	306	63.738 63.703	36.188 36.826	58.889 60.556	1.00	6.36 8.87	. :
ATOM	1675	N	HIS	307	64.186	34.026	56.808	1.00	6.09	15
ATOM	1676	CA	HIS	307	64.015	33.604	15.459	1.00	7.50	÷
ATOM	1677	CB	HIS	307	65.038	32.519	15.083	1.00	11.44	ŧ
ATOM	1678	20	HIE	207	64.853	31.183	55.746	1.30	14.32	÷
ATOM	1679	CD2		307	64.068	30.124	55.420		16.07	÷
ATOM	1680	ND1	228	307	65.704	30.723	55.734		16.54	7
atom Atom	1681 1682	CEI	HIS	307 307	65.467 64.478	29.448	55.976		14.82	÷
ATOM	1663	0	HIS	307	62.576	29.056 33.176	56.192 55.236	1.00	9.06	, 5
ATOM	1684	5	HI.S	307	61.811	32.390	56.188		11.93	à
MOTA	1685	::	PHE	308	62.167	33.136	53.980	1.00	9.50	7
MOTA	1686	ΞÀ	PHE	308	60.815	32.725	53.647	1.00	6.83	÷
MOTA	1687	CB	PHE	308	50.481	33.092	52.167	1.00	7.92	÷
ATOM	1688		PHE	308	60.530	34.55?	51.891	:.oc	5.48	÷
atom atom	1689		PHE	308	51.140	35.016	50.747	1.00	6.64	· ·
ATOM	1690 1691		PHE	308 308	59.935 61.152	35.482 36.402	52.73B 50.448	1.30	9.42	:
ATOM	1692		PHE	308	59.942	36.873	52.445	1.50	3.48 3.15	3
ATOM	1693	52	PHE	308	60.547	37.324	\$1.307	1.30	6.33	
ATOM	1694	5	PHE	308	60. 68 9		53.849	1.00	5.44	
ATOM	1695	:	PHI	308	61.489		53.322	20	5.17	:
ATOM	1696	2.	SLY	308	59.746		54.691	1.00	5.25	
ATOM	1697	24	GL Y	339	59.517		54.922	1.00	5.83	÷
ATOM ATOM	1698	:		309	50.315	28.375	54.098	1.36	6.57	
ATOM	1699 1700	Ň	SLY PF:	309 310	57.806 57.791	29.766 27.766	53.316 54.223	1.00	8.19 5.60	9 7. W. S S.
ATOM	1701	CD	PF.	310	58.486		54.742	1.20	9.04	
MOTA	1702	CA	P7.	310	56.648		53.384	1.00	9.55	
ATOM	1793	23	PF.:	210	56.581		53.449	1.00	2.33	•
ATOM	1704	23	PF.:	310	57.958	25.497	53.857		10.25	•
ATOM	1705	=	PF.:	210	55.395		53.909		9.53	•
MOTA MOTA	1706 1707		29.0	310	54.387		53.137		12.07	:
MOTA	1708	.; .;	LET	311 311	55.322 54.145		55.161	1.95	9.08	
		201			34.143	29.114	55.756	00	5.58	:

bref21	.c.pd	b		Thu	Apı	25	12	: 27 : 47	1996	23	
ATOM	1709	CЗ	LEU	311		53.83		28.437	57.080	1.00 4.34	:
MOTA	1710		LEU	311		52.83		27.277	57.127	1.00 5.54	ŧ
MOTA	1711	CD1		311		51.52		27.802	57.619	1.00 5.36 1.00 5.32	:
MOTA	1712	CD2		311		52.68		26.580 30.580	55.781 56.002	1.00 4.95	:
ATOM	1713		LEU	311		54.34		31.411	55.540	1.00 4.76	•
MOTA	1714	C N	LEU THP.	312		55.39		30.898	56.741	1.00 5.31	-
ATOM ATOM	1715 1716		THR	312		55.68		32.285	57.075	1.00 7.52	:
ATOM	1717	CB	THR	312		54.77		32.732	58.256	1.00 7.52	•
MOTA	1718	CG1		312		54.89		34.144	58.476	1.00 10.56	:
ATOM	1719		THP.	312		55.11		31.951	59.526	1.00 6.36 1.00 6.58	÷
MOTA	1720	9	THR	312		57.16		32.342	57.444 57.215	1.00 6.58	
MOTA	1721	5 }}	THR TRP	312 313		57.86 57.64		33.477	\$7.979	1.00 5.96	-
ATOM ATOM	1722 1723	CA	TRP	313		59.03		33.653	58.382	1.00 €.32	•
MOTA	1724	C3	TRP	313		59.29	94	35.032	58.992	1.00 3.13	:
ATOM	1725	CG	TRP	313		58.9		36.213	58.158	1.00 5.28	÷
MOTA	1726		TRP	313		59.6		36.779	57.066 56.682	1.00 6.34	•
MOTA	1727		TRP	313		59.03 60.8		37.968 36.403	56.382	1.00 3.66	į
MOTA	1728		TRP	313 313		57.8		37.044	58.359	1.00 4.69	•
MOTA	1729 1730		TRP TRP	313		57.9		38.103	57.488	1.00 5.00	
MOTA MOTA	1731		TRP	313		59.4		38.784	55.656	1.00 4.75	
MOTA	1732		TRP	313		61.3	01	37.222	55.350	1.00 5.62	:
MOTA	1733		TRP	313		60.6		38.398	55.004	1.00 5.72	£
MOTA	1734	•	TRP	313		59.6		32.519		1.00 3.38	•
MOTA	1735	:	TRP	313		58.9 60.8		32.186 32.216		1.0040	÷
ATOM	1736 1737	N CA	VAL VAL	314 314		61.5		31.286			•
ATOM ATOM	1738	CB	VAL	314		62.1		30.110		1.00 4.82	•
ATOM	1739		VAL	314		62.8		29.204			:
ATOM	1740	CG2	VAL	314		61.0		29.333			é é
ATOM	1741	С	VAL	314		62.6		32.192			3
ATOM	1742	0	VAL	314		63.5		32.562			-
ATOM	1743 1744	К СА	CYS CYS	315 315		63.5		33.567			
MOTA MOTA	1745	S	CYS	315		64.4		32.948			÷
ATOM	1746	č	CYS	315		64.1	191	31.82			•
ATOM	1747	CB	CYS	315		62.		34.86			
MOTA	1748		CYS	315		62.		35.82			14
ATOM	1749		LYS	316		65. 66.		33.724 33.24			•
ATOM	1750		LYS LYS	316 316		67.		32.32			
MOTA MOTA	1751 1752			316		68.		31.44			ŧ
ATOM	1753			316		69.	242	30.81			÷
ATOM	1754			316			213	31.86			÷ -
ATOM	1755			316			029 141	32.46 34.46			:
ATOM	1756		LYS	316 316			193				1
ATOM ATOM	1757 1758		PRO	217			592				
ATOM	1759			317			284		7 67.47	1 1.00 7.88	
ATOM	1760			317			344				
ATOM	176			31.	_		365		2 68.34 9 6 8.42	8 <u>1.00 6.33</u> 6 1.00 6.27	
MOTA	176			31			.381 .773				
MOTA	176. 176		PRO PRO	31.			533				; :
MOTA MOTA	_		GLN	31			105	36.8	57 65.71	1 1.00 16.42	
ATOM		6 . C		31	В		.418				
MOTA	176			31			.369				
ATOM	176						. 603				
MOTA	176 177		D GL% El GL%				.73				e :
MOTA MOTA	177		E2 GLN				.19			05 1.00 16.4	2 .
ATOM							. 27				
ATOM						71	. 90				
ATOM		4 ::	THR				. 25				-
MOTA			A THR				.39				S :
ATOM			F THP				. 23				
ATOM ATOM			G1 THR G2 THR				.86				: و
ATOM							. 75		71 54.5	51 1.00 11.1	3 :
ATOM	178	30 1	THE	40	2	69	. 14	9 38.3			
ATOM	1 170						. 77				. ā
ATCM			A TYP)4)4		. 19 5 . 69				
MOTA MOTA			S TYP)4). B:				
ATOP 4OTA			C1 TY		04		. 03		107 52.3	7700 3.7	
ATO			E1 TY		04		4.72		543 52.0	142 1.0C 2.5	90 -

bref2	lc.p	Дb		Thu	Apr 25 1	2:27:47	1996		24	
ATOM	1787	CD2	TYP	404	65.299	40.071	53.050	1.00	2.00	ą.
ATOM	1788		TYF.	404	64.992	39.918	51.710	1.00	2.00	÷
MOTA	1789	CZ	TYR	404	64.709	38.650	51.219	1.00	2.53	
MOTA	1790	ОН	TYR	404	64.447	38.463	49.891	1.00	6.21	÷
ATOM ATOM	1791	C	TYP	404	67.374	39.373	57.169	1.00	6.87	•
MOTA	1792 1793	о И	TYP.	404 405	67.459	38.477	59.006	1.00	5.71	:
MOTA	1794	CA	SER	405	67.453 67.581	40.653 41.068	57.500	1.00	7.44	7
ATOM	1795	СВ	SEP	405	68.842	41.887	58.894 59.094	1.00	7.96 9.81	f f
ATOM	1796	OG	SER	405	69.985	41.082	59.888		14.61	÷
MOTA	1797	С	SEF	405	66.332	41.863	59.305		10.09	÷
ATOM	1798	0	SER	405	66.154	43.047	58.975		10.03	÷
ATOM	1799	N	CYS	406	65.466	41.198	60.046		10.45	7
ATOM ATOM	1800	CY	CYS	406	64.220	41.789	60.452		10.00	₹.
ATOM	1802	٥	CYS	406 406	64.192 64.900	42.035 41.386	61.938		10.98	•
MOTA	1803	СВ	CYS	406	63.096	40.827	62.709 60.107		12.25 12.32	÷
ATOM	1804	SG	CYS	406	63.277	39.951	58.514		12.21	: 6
ATOM	1805	N	HIS	407	63.363	42.987	62.332		10.98	7
ATOM	1806	CA	HIS	407	63.162	43.317	63.721	1.00	8.89	5
ATOM	1807	CB	HIS	407	64.007	44.542	64.165	1.00	11.52	5
ATOM ATOM	1808 1809	CC	HIS	407	63.779	45.803	63.370		12.77	÷
ATOM	1810	ND1	HIS	40? 407	64.324	46.233	62.204		11.11	÷
ATOM	1811	CEI		467	62.968 63.025	46.832 47.837	63.812 62.954		10.97	7
ATOM	1812	NE 2		497	63.840	47.499	61.969		10.32	÷
ATOM	1813	S	HIE	407	51.687	43.614	63.801	1.00	3.26	:
ATOM	1814	Ō	HIS	407	61.078	43.935	62.789		10.54	:
ATOM	1815	N	PHE	408	61.099	43.443	64.976	1.30	7.42	7
MOTA	1816	CY	PHE	408	59.690	43.746	65.168	1.00	6.36	÷
ATOM	1817 1818	CB	PHE	408	59.281	43.636	66.643	1.00	5.63	ŧ
atom Atom	1819	CD1	PHE	408 408	59.441 59.675	42.280	67.218	1.00	3.30	6
ATOM	1820	CD2		408	59.411	42.125 41.158	68.562 66.409	1.00	4.11	5
ATOM	1821		PHE	408	59.888	40.882	69.095	1.00	4.22 2.80	÷
MOTA	1822	CE2	PHE	408	59.626	39.885	66.935	1.00	4.80	ě
ATOM	1823	CZ	PHE	408	59.866	39.751	68.282	1.00	4.71	5
ATOM	1824	C	PHE	408	59.459	45.185	64.736	1.00	6.02	5
ATOM	1825	0	PHE	408	60.370	46.018	64.744	1.00	8.84	7
atom atom	1826 1827	N CA	GLY	409	58.231	45.463	64.347	1.00	4.91	7
ATOM	1828	C	GLY	409 409	57.868 56.494	46.791 46.954	63.936	1.00	2.33	÷
ATOM	1829	ŏ	SLY	429	55.996	46.065	64.509 65.196	1.00	2.02 4.33	÷
ATOM	1830	N	PRC	410	55.879	48.100	64.299	1.00	2.00	7
ATOM	1831	CD	PRO	410	56.497	49.286	63.693	1.00	2.98	÷
ATOM	1832	CA	PRC	410	54.544	48.397	64.788	1.00	3.72	÷
ATOM	1833	CB	PP.C	410	54.276	49.754	64.166	1.00	5.67	ŧ.
ATOM ATOM	1834	CC	PRC	410	55.623	50.390	64.195	1.00	5.29	•
ATOM	1835 1836	ე ე	PRO	410 410	53.525	47.367	64.313	1.00	7.04	
ATOM	1837	N	120	411	52.831 53.471	46.752 47.165	65.137 62.987	1.00	8.58	•
ATOM	1838	CA	LEU	411	52.544	46.233	£2.329	1.00	6.97	: £
ATOM	1939	CB	LEU	411	52.254	46.674	60.898	1.00	5.66 8.28	5
ATOM	1840	CC	LEU	411	51.310	47.803	E0.553	1.00	11.17	÷
ATOM	1841		LEU	411	50.007	47.519	61.244		15.07	÷
MOTA	1842		LEU	413	51.886	49.156	60.961	1.00	14.05	÷
ATOM	1843	C C	LEO	411	53.052	44.831	62.192	1.00	4.04	-5
MOTA MOTA	1844 1845	N	LEU	411	52.365	43.870	62.481	1.00	2.7B	3
MOTA	1846	CA.	THR	412 412	54.237 54.749	44.705 43.388	61.643	1.00	3.16	-
ATOM	1847	CB	TSR	412	53.985		61.431 60.244	1.00	2.09 2.00	÷ :
MOTA	1848	0G1	THR	412	54.152	41.413	€0.166		4.84	•
ATOM	1849	CG2	THR	412	54.417		58.976	1.00	2.00	•
MOTA	1850	S	THR	412	56.252		€1.220	1.50	2.54	:
ATOM	1851	0	THR	412	56.732		£1.376	1.50	3.93	:
MOTA MOTA	1852	,, ,,	TOP	412	57.003		60.964	1.00	3.38	:
ATOM	1853 1854	CA CB	TP.P	413 413	58.468 59.003		60.747	1.00		•
ATOM	1855	CC	TRP	413	58.912		60.115 60.909	1.00	3.65 2.26	;
ATOM	1856		TT.P	413	59.722		€2.023	1.00	4.36	÷ ;
ATOM	1857		TP.P	413	59.374		62.398	1.00		
MOTA	1858	CEB	TP.P	413	60.712		62.745	1.00		4
ATOM	1859		TP.P	413	58.121	39.011	60.667	:.36		•
ATOM	1860		TF.P	413	58.395		£1.546	1.00		
ATOM ATOM	1861 1862		TPP	413	59.975		63.459	1.00	7.15	•
MOTA	1863		TEP	413 413	61.312 50.941		63.801	1.00		
ATOM	1864	C	TF:P	413	58.960		64.152 59.832	50	9.17	:
					30.500		2		5.50	77

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ATOM	1865 :	TRF	413	58.187	44.350	59.115	1.00 7.06 3
MOTA	1866 %	VAL	414	60.273	43.923	59.813 58.957	1.00 6.50 7 1.00 5.63 f
MOTA	1867 C		414	60.904 61.078	44.921 46.289	19.660	1.00 7.88
ATOM	1868 C3	VAL	414 414	62.193	47.072	59.029	1.00 6.76
ATOM ATOM		2 VAL	414	59.789	47.111	59.547	1.00 3.37 5
MOTA	1871 C 1872 C	VAL	414	62.242	44.340	58.533	1.00 9.59 5
MOTA		VAL	414	63.183	44.296 43.820	59.303 57.314	1.00 9.75 7
ATOM	1873 :	CYS CYS	415 415	62.296 63.515	43.222	56.809	1.00 9.19 5
ATOM	1874 C	CYS	415	64.238	44.007	55.767	1.00 9.05
Mota Mota	1876 C	CYS	415	63.714	44.949	55.189	1.00 8.76 3
MOTA	1977 6	B CYS	415	63.207	41.882	56.222	1.00 3.11 ÷ 1.00 14.13 1÷
MOTA	1878 5		415	62.067	41.071 43.622	57.341 55.581	1.00 7.88
ATOM	1879 N		416 416	65.484 66.341	44.197	54.585	1.00 9.50 5
MOTA	1880 C	h LYS B LYS	416	67.175	45.349	55.135	1.00 14.71 5
atom atom	-	S LYS	416	66.482	46.235	56.144	1.00 19.54 5
ATOM		D LYS	416	66.618	45.629	57.541	1.00 23.24 6 1.00 23.74 6
MOTA		E LYS	416	65.851	46.404	58.599 59.937	1.00 23.74 6
MOTA		Z LYS	416	66.292 67.234	45.088 43.008	54.278	1.00 12.10 5
ATOM	1886 C		416 416	67.523	42.187	55.175	1.00 10.95 ê
MOTA MOTA	1888		417	67.573	42.817	52.990	1.00 12.45
ATOM		D PRO	417	67.231	43.561	51.771	1.00 11.38 ÷
ATOM		A PRO	417	68.434	41.684	\$2.671 \$1.144	1.00 11.76 5 1.00 10.58 5
ATOM		B PRO	417 417	68.394 68.247		50.780	1.00 11.41
MOTA MOTA		CS PRO	417	69.845		53.221	1.00 14.43
ATOM		PRO	417	70.361		53.325	1.00 14.95 \$ 1.00 15.69 7
ATOM		N GLN	418	70.400			- · · · · · · · · · · · · · · · · · · ·
ATOM		CA GLN	418	71.753			
MOTA		C3 GLN	418	71.933 71.948			
ATOM		CG GLN	418 418	71.580			1.00 16.21 5
MOTA MOTA		OE1 GLN	418	71.377			
ATOM		NE2 GLN	418	71.478			
MOTA		C GLN	418	72.660			
MOTA	1903	C GLN	418	72.470 36.63			
ATOM	1904 1905	% LYS	510 510	36.98			1.00 22.39
MOTA MOTA	1906	CB LYS	510	37.00	4 45.50		1.00 22.50
ATOM	1907	CS LYS	510	37.79		9 100.099	
ATOM	1908	CD LYS	510	39.38 40.14		6 99.984 B 101.30	
ATOM	1909	NZ LYS	510 510	40.14	-	7 101.71	0 1.00 21.46
MOTA MOTA	1910 1911	C LYS		36.03	9 43.64	2 97.54	2 1.50 21.11 🗧
ATOM	1912	LYS		26.11			
Atom		: PHE		35.08			
MOTA		CA PHE		34.20 32.90			
MOTA		CB PHE		31.96			2 1.00 17.36 5
ATOM ATOM		CO1 PHI		32.47	0 40.35		
ATOM		CO2 PH		30.59			5 1.00 19.23 5 9 1.00 16.04 f
ATOM	1919	CE1 PH		31.63			
ATOM		CE2 PH		29.73 30.2			
ATOM ATOM		CZ PH		35.0			4 1.00 17.52 5
ATON		PH		25.4			
ATO	1 1924	: GL		35.4			92 1.00 17.14 1 16 1.30 18.20 5
ATO		CA GL		36.2 36.5			
ATON	_	OF GL		37.4			75 1.00 28.00
OTA OTA		SS GL		36.8		87 90.10	01 1.00 30.11
ATO		III GL	C 512	37.3			
ATO	M 1930	:E2 G1	.U 512	35.8			
ATO		: GI		37.5 37.9			6130 15.76
ATO		y SI		37.9		63 94.9	30 1.20 13.17
ATO		CA SI		39.3	34 42.0	08 95.7	
• ATO	M 1935	CF 51	R 512	39.5			
ATO			ER 513	40.3 39.3			
ATC ATC			ER 513 ER 513	40.0			
ATO			YS 514	38.		97.5	37336 11.94
ATC	M 1940	th L	YS 514	37.			
ATC			YS 514	36.	839 40.	12: 59.(
ATC	M 1942	: 25 L	YS 514	3".	238 41	165 100.	627 1.30 3.11

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ATOM	1943	CD	LYS	514	36.388	41.093	101.842	1.00 2.00	:
ATOM	1944	CE	LYE	514	36.374		102.539	1.00 2.00	÷.
MOTA	1945	NZ	LYS	514	35.665		103.798	1.00 3.28	;
ATOM	1946	С	LYS	514	37.621	38.443	97.959	90 11.50	:
MOTA	1947	0	LYS	514	37.841	37.435	98.620	1.00 13.26	÷
ATOM	1948	К	ALA	\$15	37.138	36.401	96.716	1.00 10.50	.
ATOM	1949	CA	ALA	515	36.876	37.117	96.038	1.00 9.26	₹
ATOM	1950	CB	ALA	515	36.187	37.366	94.719	1.00 10.39	•
ATOM	1951	c	ALA	515	38.165	36.299	95.806	§5.6 00	•
ATOM	1952	0	ALA	515	38.176	35.068	95.920	1.00 7.78	÷
ATOM	1953 1954	N CA	ALA	516	39.241	37.026	95.494	1.00 8.76	-
ATOM ATOM	1955	CB	ALA ALA	516 516	40.562 41.457	36.478 37.533	95.204	1.00 7.65	÷
ATOM	1956	c	ALA	516	41.205	35.872	94.614 96.419	1.00 6.46 1.00 7.37	÷
ATOM	1957	õ	ALA	516	41.690	34.751	96.353	1.00 7.37 1.00 8.85	÷
ATOM	1958	N	LEU	517	41.226	36.599	97.530	1.00 8.63	÷
ATOM	1959	CA	LEU	517	41.809	36.040	98.743	1.00 5.52	į
ATOM	1960	CB	LEU	517	41.445	36.874	99.947	1.00 3.15	5
ATOM	1961	CG	LEU	517	42.141	38.193	100.158	1.00 4.53	÷
ATOM	1962		LEU	517	41.717	39.177	99.108	1.00 9.66	5
ATOM	1963		LEU	517	41.754	38.683	101.519	1.00 4.29	5
ATOM	1964	Ç	LEU	517	41.271	34.634	98.992	1.00 7.39	સ
ATOM	1965	C	LEU	517	42.009	33.751	99.437	1.00 10.93	÷
ATOM	1966	N	LEU	518	39.997	34.433	43.648	1.00 3.49	7
ATOM	1967	CA	LEU	518	39.297	33.177	98.857	1.00 7.25	÷
ATOM	1968	CB	LEU	51B	37.845	33.467	99.273	1.00 5.35	₹.
MOTA	1969	CG.	LEU	51 B	37.614		160.773	1.00 5.58	÷
MOTA	1970		LEU	516	36.802		100.936	1.00 3.48	
MOTA MOTA	1971 1972	CD2	LEU	518 518	36.951 39.239		101.495	1.00 6.87	5.
MOTA	1973	ō	LEU	518	39.185	30.955	97.733	1.00 9.11	5
ATCM	1974	N	ALA	519	39.557	32.623	97.979 96.505	1.00 8.10 1.00 11.23	E 7
ATOM	1975	CA	ALA	519	39.603		95.342	1.00 13.35	5
ATOM	1976	CB	ALA	519	39.310		94.072	1.00 12.74	5
ATOM	1977	C	ALA	519	40.908		95.209	1.00 15.14	÷
ATOM	1978	C	ALA	519	41.733		94.311	1.00 15.55	Ė
ATOM	1979	N	ALA	520	41.047		96.068	1.00 17.93	7
MOTA	1980	CA	ALA	520	42.228	29.064	96.115	1.00 19.81	÷
ATOM	1981	CB	ALA	520	42.169	28.165	97.371	1.00 20.83	÷
ATOM	1982	C	ALA	520	42.579		94.865	1.00 19.53	÷
ATOM	1983	9	ALA	520	41.764		94.339	1.00 19.29	:
ATOM	1984	N	ARG	521	43.834		94.449	1.00 90.00	7
ATOM	1985	CA	ARG	521	44.407		93.322	1.00 90.20	•
ATOM	1986	C3	ARG	521	45.499		92.652	1.00 90.00	•
ATOM ATOM	1987 1988	CG	ARG ARG	521 521	45.117 45.751		92.441 93.500	1.00 90.00	÷
ATOM	1989	NE	ARG	521	45.512	30.871 30.373	94.854	1.00 90.00	•
ATOM	1990	CZ	AP.G	521	46.279		95.464		•
MOTA	1991		ARG	521	47.351		94.843	1.00 95.00	;
ATOM	1992	NH2		521	45.888		96.620	1.00 90.00	.
MOTA	1993	c	ARG	521	45.018		93.866	1.00 90.30	÷
ATOM	1994	0	ARG	521	44.842	26.022	95.032	1.00 90.00	Ē
ATOM	1995	Ņ.	GLY	522	45.710	25.592	93.022	1.00 90.30	-
MOTA	1996	CA	GLY	522	46.338		93.500	1.00 90.00	÷
MOTA	1997	ε	GLY	522	47.851		93.549	1.00 90.00	÷
ATOM	1998	Č.	GLY	522	48.286		93.891	1.00 90.10	•
ATOM	1999	, c.	PRO	523	18.672		£3.225	30 93.00	
ATOM ATOM	2000 2001	CY CD	PRC-	523 523	48.070 50.157		92.929	1.00 90.00	÷ :
MOTA	2002	CB	PRO	523	50.429		93.185 92.201	1.00 90.00	4
ATOM	2003	CG	PRO	523	49.27		92.486	1.00 90.00 1.00 90.00	÷
ATOM	2004	S	PRO	523	50.968		92.741	1.00 90.00	•
ATOM	2005	š	PRC	523	50.499		91.984	1.00 93.30	- :
ATOM	2006	N	SLU	524	52.22		93.180	1.00 24.71	:
ATCM	2007	Ç,	SLT	524	53.12		92.829	00 23.63	Ŀ
ATOM	2008	CF	GL:	524	54.28			1.00 27.67	÷
ATOM	2009	CS	GLU	524	55.48		93.730	00 27.39	
ATCM	2013	CD	GLU	524	55.20		94.250	1.00 31.35	:
ATOM	2611	OEI	GL:	524	54.91			1.00 23.10	•
MOTA	2012	OE 2	CLU	524	55.34	3 23.263		00 31.26	•
ATOM	2013	ć	GLU	524	53.67	25.532	91.428	1.00 21.32	
MOTA	2014	÷.	CLU	524	53.70			1.00 25.22	•
ATOM	2015): 	GLU	525	54.16			1.00 18.30	
MOTA MOTA	2016 2017	CA	GLU	525	54.72			1.06 13.58	:
ATOM	2017	CB	GLU	525 525	53.55			1.00 18.50	:
ATOM	2019	CD	GLU	525	53.85 52.59			1.00 27.12	•
ATOM	2020		GLU	525	52.47			1.00 31.94	;
								00 34.45	,

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ATOM	2021	OE2	GLU	525	51.		26.066			.00 34.1		
MOTA	2022	С	GLU	525	55. 55.		27.633			1.00 B.		
MOTA	2023	C	GLU LEU	525 526		619	27.49			00 5.	J	
ATOM	2024 2025	N CA	LEU	526		455	28.63	8 87		1.00 4.		
ATOM ATOM	2025	CB	LEU	526	58.	859	28.18			30 4.		
ATOM	2027	CC	LEU	526		103	29.08				00 ÷	
ATOM	202B		LEU	526		166	28.50 30.49	_	5.706 7.193		00	
MOTA	2029		LEU	526 526		856 688	29.24		5.751		64	
ATOM	2030 2031	0	LEU	526		527	28.60	7 8	5.733		a0 :	
MOTA MOTA	2032	N	LEU	527		209	30.47		6.892		.00 :	
ATOM	2033	CA	LEU	527		415	31.10		5.854 6.441		.00 f	
MOTA	2034	CB	LEU	527 527		.115	31.63 30.65		6.824		. 65	
MOTA	2035 2036	CG	LEU	527		. 951	31.42		7.441		.00	
Mota Mota	2037		LEU	527		.547	29.88		5.620		.00 =	
ATOM	2038	С	LEU	527		.110	32.25		5.176		.04 :	
ATOM	2039	0	LEU	527		.413	33.25	_	5.836 3.844		.30 · · · · · · · · · · · · · · · · · · ·	
ATOM	2040	N CA	CYS	528 528		. 929	33.1		3.051		.97 :	
MOTA MOTA	2041 2042	c	CYS	528		.987	33.8	10 8	2.044		.18	
ATOM	2043	ō	CY5	528		.087	33.1		1.560		.61	
ATOM	2044	СВ	CYS	528		.132	32. 5 31.8		2.282 3.234			
MOTA	2045	SG	CYS	528		.491	35.0		1.743		.00	
MOTA	2046	N	PHE PHE	529 529		. 397	35.7		0.758		.15	
ATOM ATOM	2047 2048	CA CB	PHE	529		.008	36.1		21.303	1.00 3	. BB .	
MOTA	2049	CG	PHE	529		. 980			22.231		2.00	
MOTA	2050	CD	1 PHE	529		3.958			61.733		2.00	
ATOM	2051		2 PHE	529		3.912 3.868	_		63.611 62.590		2.00	
ATOM	2052		1 PHE 2 PHE	529 529		3.822			84.471		2.00	
ATOM ATOM	2053 2054					3.801		90	E3.961		2.00	
ATOM	2055		PHE		5	6.100			80.200		5.77 f 6.52 =	
ATOM	2056		PHE		_	7.078			80.785 79.018		6.52 = 2.84	
MOTA	2057		THE			5.665 6.225			78.377		2.00	
ATOM	2058 2059				_	7.228			77.232	1.00	2.00	
MOTA MOTA	206		1 THE		_	7.683			76.579		2.84	
ATOM	206				_	6.63			76.234		2.96 ÷	
MOTA	206		THE		0 5	5.07 3.99	6 39. 9 39.		77.948 77.611		4.31	
ATOM	206		TH			5.27			78.076		4.43	
MOTA MOTA	206 206				_	4.24	6 41.	854	77.747	1.00	5.46	
MOTA	206			y 53	:	4.17		913	73.836		0.50	:
MOTA	206				-	54.04		346 413	80.257 81.298			:
ATOM	206		D GL El Gl			53.77 54.08		606	£1.079		15.54	:
MOTA	206 207		E2 GL			53.22	i	052	£2.35	5 1.00	18.13	•
MOTA MOTA					11	54.46	-	489	76.38			:
ATOM		2 0	GL		-	53.50		. 685	75.650 76.15		9.10 5.91	•
ATOM					_	55.65 56.0:		. 021 . 52 9	74.83			•
ATOM			a Af			56.90		. 795	74.89	0 1.00		÷
atom Atom			G AF		32	56.14	41 46	.059	75.09		4.16	:
ATOM			IA C			55.6		.070	76.46 76.69		6.94 14.70	:
ATOM	-	78 ' t			32	54.5		.930 .395	77.89		17.72	:
ATOM		-	CZ AI NH1 AI		32 32	54.B		.096	73.97	5 1.00	13.74	
MOTA MOTA			NH2 A	RG 5	32	52.9	98 48	.056	73.01		18.08	•
ATO				RG 5	32	56.9		. 364	74.43	4 1.00	9.68 12.29	:
ATO	4 20				32	56.9		.310	75.05 73.43		10.64	
ATO					22 23	57.7 58.6		356	73.19	500	12.12	
ATO					23	58.3		. 790		21 1.00	13.13	
OTA OTA				EU S	33	56.8	84 40	. 298	71.74	11 1.00	10.95	
ATO		88	CD1 L	EU 5	23	56.5		2.773	70.3		11.69 12.40	
ATO	M 20		CD2 L		23	56.7		9.204 1.733			12.40	
ATO		90			123 523	60.6		1.590			12.70	
ATO ATO)91)92			534	60.	365 4	2.115	74.6	66	12.95	
ATO		93	Ch C	il: :	534	61.		2.523			13.30	
ATC	M 20	94			534	61.		3.822 4.974			16.94 23.38	
ATC		95			524 534	51.60.		6.010			26.3	
ATC ATC		096 097	CD (534	59.		€.86	73.8	62 1.00	26.36	
ATC		098	DE2		534	61.		5.93	72.6	25	25.83	

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MOTA	2099	С	GLU	534	61.892	42.579	75.527	1.00 10.35
ATOM	2100	C	GLU	534	62.651	42.380	₹7.066	1.00 10.92
ATOM	2101	N	ASP	535	61.251	41.637	77.194	1.00 9.01 ;
ATOM	2102	CA	ASP	535	61.247	41.578	78.638	1.00 6.92 {
atom Atom	2103	CB	ASP	535	60.188	42.544	73.128	1.00 8.31 €
ATOM	2104 2105	CG	ASP ASP	535 535	58.848 58.020	42.334	78.430	1.00 8.75 4
ATOM	2106		ASP	535	58.635	41.541 42.949	78.913 77.372	1.00 11.89 :
ATOM	2107	c	ASP	535	60.793	40.201	79.033	1.00 15.77 £
ATOM	2108	C	ASP	535	60.062	39.577	73.295	1.00 6.65
MOTA	2109	N	LEU	536	61.178	39.731	89.204	1.00 5.28 7
ATOM	2110	Ch	LEU	536	60.717	38.436	80.651	1.00 4.48 -
ATOM	2111	CB	LEU	536	61.614	37.315	80.149	1.00 2.00 5
ATOM	2112	CG	LEU	536	61.012	35.958	80.495	1.00 2.00 4
atom Atom	2113 2114		LEU	536 536	59.697 61.955	35.789 34.853	73.782	1.00 2.00 €
ATOM	2115	C	LEU	536	60.725	38.468	80.152 82.154	1.00 2.00 6
ATOM	2116	ō	LEU	536	61.701	38.896	82.751	1.00 5.42 6 1.00 5.81 8
ATOM	2117	N	VAL	537	59.606	38.093	82.767	1.00 6.59 7
MOTA	2118	CA	VAL	537	59.514	38.050	84.219	1.00 4.71 6
ATOM	2119	CB	VAL	537	58.439	39.006	84.761	1.00 3.90 6
ATOM	2120		VAL	537	58.391	38.900	B6.262	1.00 7.66 5
atom atom	2121 2122		VAL	537	58.754	40.434	E4.386	1.00 6.66
ATOM	2123	0	VAL	537 537	59.111 58.232	36.652 36.096	£4.604	1.00 2.70 4
ATOM	2124	N	CYS	538	59.812	36.048	83.977 85.553	1.00 5.62 ± 1.00 3.31 T
ATOM	2125	CA	CYS	538	59.452	34.711	E5.055	1.00 3.31 7 1.00 4.73 4
ATOM	2126	С	CYS	538	59.375	34.771	87.597	1.30 5.86 6
ATOM	2127	٥	CYS	538	60.165	35.457	£3.257	1.00 6.30 8
ATOM	2128	CB	CY5	538	60.438	33.619	E5.600	1.00 2.00 €
MOTA	2129	SG	CYS	538	60.634	33.421	83.795	1.00 3.79 16
atom atom	2130 2131	N CA	PHE	539 539	58.426	34.059	88.178	1.06 3.78 7
ATOM	2132	CB	PHE	539	58.267 57.295	34.099 35.232	89.621	1.00 4.15 6
ATOM	2133	CG	PHE	539	55.852	35.009	89.997 89.515	1.00 4.88 6 1.00 7.86 6
ATOM	2134		PHE	539	54.835	34.690	90.420	1.00 5.60 6
ATOM	2135	CD2	PHE	539	55.519	35.104	88.147	1.00 9.65 6
ATOM	2136	CE1	PHE	539	53.540	34.470	89.986	1.00 4.81 5
ATOM	2137		PHE	539	54.201	34.878	87.706	1.00 7.22 5
ATOM	2138	cz	PHE	539	53.223	34.562	88.630	1.00 5.52 5
atom Atom	2139 2140	0	PHE	539	57.689	32.807	90.123	1.00 3.30 €
ATOM	2141	N	TEF	539 540	57.397 57.606	31.913 32.696	29.352	1.00 5.07 3
ATOM	2142	CA	TRP	540	56.965	31.575	91.436 92.102	1.00 2.62 7 1.00 5.41 6
ATOM	2143	CB	TRP	540	57.859	30.331	92.252	1.00 5.13 €
ATOM	2144	CG	TP.P	540	58.890	30.380	93.315	1.06 7.06 4
ATOM	2145	CD2	TRP	540	60.250	30.807	93.175	1.50 4.64 5
ATOM	2146	CE2	TPP	540	60.861	30.65?	94.430	1.50 5.73 4
atom Atom	2147	CE3	TPP	540	61.008	21.299	92.110	1.00 5.86 5
ATOM	2148 2149	CD1 NE1	TRP TRP	540 540	58.738 59.914	29.995	94.610	1.56 8.29 4
ATOM	2150		TRP	540	62.208	30.161 30.984	95.286 94.657	1.00 8.36 7
ATOM	2151		TPP	540	62.336	31.623	92.328	1.00 8.15 5 1.00 7.58 5
ATOM	2152		TP.P	540	62.927	31.465	93.596	1.00 8.06 5
ATOM	2153	Ç	TRP	540	56.504	32.189	93.417	1.00 6.24 5
ATOM	2154	٥	TPP	546	56,774	33.366	93.668	2.00 7.32 3
MOTA	2155	19	CLU	541	\$5.698	31.467	94.186	1.00 8.81 7
MOTA	2156	, CY	GLU	541	55.187	31.399	95.452	1.00 10.45 ÷
mota Mota	2157 2158	CB	GLU	541 541	53.768	32.565	95.270	1.00 11.89 4
MOTA	2,59	CD	CTA	541	53.592 52.202	33.523 34.134	94.070 93.991	1.00 14.89 5
ATOM	2160		GLU	541	52.094	35.229	93.415	1.50 16.24 4 1.50 17.33 A
MOTA	2:61		GLU	541	51.219	23.550	94.516	1.30 16.64 3
ATOM	2:62	C	GLU	541	55.148	30.925	95.507	1.50 10.03 4
MOTA	2:53	?	GLU	541	54.744	29.811	95.232	1.00 10.32
ATOM	2164	N	GLU	542	55.552	31.242	97.724	1.50 10.91 1
MOTA MOTA	21.65	CA	GLU	542	55.521	30.222	93.766	1.00 10.78 5
ATOM	2166 2167	CE	GLU	542 542	56.971 59.122	29.482 30.359	98.833 98.738	1.00 10.24 5
ATOM	2168	CD	SLU	542	59.400	29.571	99.306	1.00 14.40 6 1.00 15.97 6
MOTA	2169	OE1	GLU	542	59.711		100.188	1.00 17.03
ATOM	2170		GLU	542	60.095	29.263	98.026	1.00 17.30 3
ATOM	21.71	2	GLU	542	55.C83		166.128	9.66
ATOM	2172	2	GLU	542	54.741	31.947	100.248	1.00 9.as 4
ATOM	2173	33	ALA	543	55.951		101.135	1.00 €.31 "
atom Atom	2174 2175	CA CB	ALA ALA	543	54.652		102.493	1.50 7.10 4
ATOM	2176	C	ALA	543 543	54.466 55.716		103.325	1.00 4.26 4
		-	nun	24 D	55.716	21.141	103.108	1.00 8.66 3

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ATOM	2177	٥	ALA	543	5	6.91	1 3	0.849	102.	998	.00 10		:
ATOM	2178	N	ALA	544		5.28		2.253		695	00 9 00 10		
MOTA	2179	CA	ALA	544		6.19		3.185 4.374			1.00 10		
ATOM	2180	CB	ALA	544		55.42 56.86		2.397			1.00 11		
MOTA	2181	S	ALA	544 544		56.16	_	3.744			00 13		!
MOTA MOTA	2102 2183	0	SER	545		58.20	4 3	2.393	105.	456	00 12		
MOTA	2184	CA	SER	545		58.99		1.669			1.00 13	.08	£
ATCM	2185	CB	SER	545		59.33		0.25i 29.628			1.00 12	.06	€ ÷
ATOM	2186	OG	SER	545 545		60.29 60.24		2.440			1.00 14		ŧ
MOTA	2187	c c	SEP. SER	545		60.86		33.184			1.00 15	. 67	:
ATOM ATOM	2188 2189	N	ALA	546		60.5	57 3	32.271			00 17	.50	-
ATOM	2190	CA	ALA	546		61.63		32.942			1.00 17		į.
ATOM	2191	CB	ALA	546		61.9	_	32.215 33.213			1.00 17		•
HOTA	2192	c	ALA	546 546		62.9		32.297			1.00 19		ā
MOTA	2193	C N	ALA GLY			63.2	-	34.495			1.00 19		-
atom atom	2194 2195	CA	GLY			64.4	38	34.8B9	167	.360	:.00 20		÷
ATOM	2196	c	GLY			64.8		34.140			1.00 20	3.86	5
ATOM	2197	O	GLY			66.0		34.046			1.00 2		=
ATOM	2198	N	VAL			63.8		32.560			1.00 1		Ę
MOTA	2199	CA CB	VAL VAL	_		64.1		31.74			1.00 1		ŧ
ATOM ATOM	2200 2201		VAL VAL			63.1	_	31.30	9 102	2.363	1.00 1	3.62	5
ATOM	2202		2 VAL			63.4		30.57			1.00 1		ŧ ş
ATOM	2203		VAI			63.8		33.97			1.00 1	5.33 6.13	
ATOM	2204		VAI			62.7 64.9		34.30			1.00 1	5.42	:
ATOM	2205		GL)			64.8		35.66			1.00 1		£
MOTA MOTA	2206 2207		GLY			65.4		35.18	0 10	0.263	1.00 1	2.73	5
ATOM	2208		GL	-		65.	765	33.99			1.00 1		;
ATOM	2209	N	PR			65.		36.06		9.283 9.166	1.00 1		É
MOTA	2210					65.		37.45 35.63		3.017	1.00 1		5
ATOM	2211					66.		36.94		7.199	1.00		5
MOTA MOTA	2212 2213			-		66.		38.01		8.199	1.00 1		÷
MOTA	2214		PR			67.	647	34.96		8.157	1.00		•
MOTA	221		PR			67.		34.00		7.377	1.00		3.7
MOTA	221		GL				384 714	35.34 34.79		9.204	1.00		4
ATOM	221		GL GL				776	33.30		9.601	1.00	9.01	We sto the story
MOTA MOTA	221		GL				854	32.7		9.588		11.57	:
ATOM	222	-	λS			68.	625	32.6		3.726		6.84	-
ATOM	222						573	31.2		9.888		6.10 4.08	÷
MOTA	222						510 797			.).904 2.226		6.03	•
ATOM			G AS				789			2.850		7.24	3
MOTA MOTA			D2 AS				991		11 10	2.631	1.00	3.39	•
ATOM				SN 5	32		. 287	30.5		98.590		7.54	÷
ATOM		7 C		5N 5			.176	29.2		98.580 62.504		7.91 5.28	5
MOTA					53		.157 .867	31.2 30.7		97. 5 06 94.186		4.43	;
ATOM					53 53		.432	31.0		95.779		4.87	÷
ATOM ATOM					53		.367	30.3	41	95.520		4.46	•
ATOM			D1 T	YP. 5	53	64	.491			\$7.37		3.71	:
ATOM	223	33 C	E1 T		53		.574			93.11°		3.40 3.40	
ATOM			D2 T		53 53		.280 .355			37.16		3.44	÷
MOTA			E2 T		53 53		.516			93.01		2.00	:
ATOP ATOP					53	62	. 650	28.	183	35.77	8 1.30	3.67	•
MOTA				YR 5	53		1.791			35.11			•
RTO		-			.53		. 432			25.29			-
ATO					.54 :54		9.845 9.622			12.98 12.3€			:
ATO:					:54 :54		0.999			32.33	2 1.00	3.42	:
ATO ATO					54		0.954	4 29.	192	\$2.21	4 1.00	11.53	•
ATO					554	68	8.800	30.	783	31.62			
ATO	M 22	45	o :	SEF.	54	-	8.28		584	21.50			
ATO					555		e.574 7.81		783 640	99. 7 7 89. 5 3			
ATO					555 555		6.73		730	23.48			
ATO ATO					:55		5.78	C 32.	595	88.33	25	: :.∋9	ı
ATO			CD1 :	PHE	555		4.42		509	85.50			
ATC	24 22	251	CD2		555		6.24		354	87.00 87.50			
ATC		252	CE1 CE2		558 555		3.54		. 382 . 427	25.9			
ATC ATC		253 254		PHE	555		4.03		339	85.1			

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ATOM	2255	С	PHE	555	68.779	31.759	E8.337	1.00 6.86	÷
ATOM	2256	þ	PHE	555	69.184	32.858	87.945	1.00 8.43	•
ATOM	2257	N	SER	556	69.095	30.616	£7.740	1.90 7.22	;
ATOM	2258	CA	SER	556	70.019	30.503	86.619	1.00 6.83	÷
MOTA	2259	CB	SER	556	70.969	29.315	86.879	1.00 4.30	÷
atom Atom	2260 2261	0G	SER SER	556 556	71.923 69.336	29.587	87.891	1.00 8.78	•
ATOM	2262	0	SER	556	68.535	30.298 29.389	85.257 85.117	1.00 5.62 1.00 8.35	÷ :
ATOM	2263	N	TYR	557	69.682	31.102	84.255	1.00 8.35	7
ATOM	2264	CA	TYP.	557	69.123	30.943	62.924	1.00 3.30	÷
ATOM	2265	CB	TYP.	55?	68.198	32.089	82.569	1.00 2.00	ŗ,
ATOM	2266	CG	TYP	557	68.832	33.434	82.422	1.00 2.00	-
ATOM	2267	CD1	TYP.	557	69.405	33.825	81.218	1.00 2.00	5
MOTA	2268	CEI	TYP.	557	69.851	35.126	€1.023	1.00 2.56	÷
MOTA MOTA	2269 2270		TYR TYR	557 557	68.737 69.184	34.368	83.434	1.00 2.00	5
ATOM	2271	cz	TYR	557	69.734	35.667 36.047	83.260 82.051	1.00 2.00	÷
MOTA	2272	ОН	TYR	557	70.124	37.356	81.865	1.00 3.10 1.00 3.23	6 3
MOTA	2273	c	TYR	557	70.191	30.834	81.870	1.00 3.33	÷
MOTA	2274	0	TYR	557	71.316	31.196	82.090	1.00 4.25	8
ATOM	2275	N	GLN	55B	69.839	30.360	80.695	1.00 3.52	ר
ATOM	2276	CA	GLN	55B	70.831	30.227	79.648	1.00 3.20	÷
atom Atom	2277 2278	CB	GLN	558	71.603	28.925	79.828	1.00 3.66	•
ATOM	2279	CD	GLN GLN	558 558	72.506	28.598	78.648	1.00 6.55	÷
ATOM	2280	OE1	GLN	558	73.171 72.552	27.282 26.320	73.788 79.163	1.00 5.14	•
ATOM	2281		GLN	558	74.447	27.229	78.477	1.90 7.23	7
ATOM	2282	S	GLN	558	70.204	36.208	73.279	1.50 3.24	
ATOM	2283	0	GLN	558	69.420	29.309	77.977	1.00 2.96	3
ATOM	2284	N	LΣU	559	70.518	31.189	77.445	1.00 2.00	7
ATOM	2285	CA	LEU	559	69.945	31.139	76.120	1.00 2.89	÷
ATOM	2286	CB	LEU	559	70.036	32.487	75.399	1.00 2.00	÷
ATOM ATOM	2287 2288	CG	LEU	559	68.975	33.527	75.792	1.00 2.00	6
ATOM	2289		LEU	559 559	69.103 67.612	34.810 32.955	75.005 75.564	1.00 2.00	5 5
ATOM	2290	c	LEU	559	70.764	30.060	75.447	1.00 2.00	5
MOTA	2291	0	LEU	559	71.951	29.947	75.728	1.00 4.67	ă
MOTA	2292	N	GLU	560	70.091	29.169	74.718	1.00 6.97	7
ATOM	2293	CA	GLU	560	70.737	28.064	73.997	1.00 11.03	5
ATOM	2294	CB	GLU	560	69.787	27.517	72.938	1.00 14.40	÷
ATOM ATOM	2295 2296	CG	GLU	560	70.290	26.305	72.163	1.00 19.08	á
MOTA	2297	OE1	GLU	560 560	69.701 69.790	26.207 27.202	70.738 69.983	1.00 20.20	÷
MOTA	2298	OE2		560	69.200	25.130	70.346	1.00 21.83	į
MOTA	2299	C	GLU	560	71.995	28.572	73.310	1.00 11.71	ě
MOTA	2300	0	GLU	560	71.919	29.491	72.505	1.00 10.88	3
MOTA	2301	N	asp	561	73.140	27.970	73.648	1.00 12.36	-
ATOM	2302	CÀ	ASF	561	74.460	28.345	73.118	1.00 13.20	÷
MOTA	2303	CB	ASP	561	74.478	28.398	71.589	1.00 11.29	÷
atom Atom	2304 2305	CG	ASP	561	74.440	27.038	70.968	1.00 13.29	•
ATOM	2306	OD2	ASP ASP	561 561	74.530 74.296	26.039 26.963	71.725 69.729	1.00 14.53	
ATOM	2307	c	ASP	561	74.995	29.667	73.661	1.00 17.27	ē.
ATOM	2308	ō	ASP	561	75.663	30.426	72.931	1.00 21.27	3
ATOM	2309	N	GLU	562	74.714	29.972	74.926	1.00 17.40	7
ATOM	2310	Cλ	CLT.	562	75.22C	31.218	75.504	1.00 16.45	÷
MOTA	2311	CB	GLU	562	74.093	32.235	75.652	1.30 20.22	÷
ATOM	2312	, CG	GLC	562	73.224	32.450	74.408	1.00 23.17	÷
atom Atom	2313 2314	CD	GLU	562 562	73.909 74.330	33.234	73.289	1.00 23.82	÷
ATOM	2315		GLU	562	73.981	34.407 32.670	73.511 72.169	1.00 22.18	3
ATOM	2316	5	SLU	562	75.764	30.847	75.871	1.30 14.28	-
HOTA	2317	•	GLU	562	75.431	29.759	77.373	1.3C 15.04	•
ATOM	2318	N	PRO	563	76.662	31.581	77.465	1.00 11.29	:
ATOM	2319	ÇD	PP.:	5.63	77.200	23.000	77.084	1.00 11.69	:
ATOM	2320	CA	PEC	563	77.156	31.287	73.794	1.30 11.69	:
MOTA MOTA	2321 2322	CR	PRC PRC	563 563	78.186 77.655	32.376	79.111	30 7.10	9 q
ATOM	2323	C	PRC	563	75.965	33.548 31.277	73.404 73.788	1.30 5.79 1.30 10.73	:
ATOM	2324	5	PRC	563	74.981	32.001	79.558	1.20 11.36	;
ATOM	2325	N	TEP	564	75.995	30.362	80.772	1.00 8.20	-
ATOM	2326	CA	TPP	564	74.945	30.255	81.806	1.00 5.30	•
ATOM	2327	CB	TF.F	564	75.304	29.199	62.845	1.11 2.55	:
ATOM	2328	CC	TRE	564	74.650	27.885	E2.700	1.00 5.08	:
ATOM ATOM	2329 2330		TRF	564 564	73.27€	27.585	82.941	6.62	•
MOTA	2331		TRE	564 564	73.116 72.158	26.188 28.357	£2.761 £3.29€	1.00 6.96	•
MOTA	2332		TP.F	564	75.250	26.700	82.38?	6.39	;
							-		•

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ATOM	2333	NE1		564		4.33		25.6		82.422 82.929	i. 1.		5.36 5.49	: :
MOTA	2334	CZZ		564 564		11.86 70.92		25.5 27.5		83.461			5.79	÷
ATOM	2335 2336	CZ3 CH2		564		0.80		26.		83.279		GO 3	3.18	÷
atom Atom	2337	c	TRP	564		14.81		31.		62.525			5.66	₹ •
ATOM	2338	C	TRP	564		75.9		32.		82.740			9.32 3.69	:
MOTA	2339	N	LYS	565		73.6: 73.5		31.5		82.927 83.612			2.30	•
MOTA	2340	CB	LYS	565 565		73.0		34.		62.625			2.50	Ę
atom Atom	2341 2342	CG	LYS	565		74.2		34.		81.791	1.		2.20	:
ATOM	2343	CD	LYS	565		73.8		35.		E0.371			3.81	÷
MOTA	2344	CE	LYS	565		74.B		36. 37.		79.711 80.497			3.15 6.31	÷
ATOM	2345	NZ C	LYS LYS	565 565		74.8 72.6			171	84.878			3.24	÷.
ATOM ATOM	2346 2347	ŏ	LYS	565		71.8			270	85.043			2.93	:
ATOM	2348	N	LEU	566		72.8			113	85.783			3.46	,
ATOM	2349	CA	LEU	566		72.1			100 857	87.042 88.143		. 00 . 00	5.16 7.13	
MOTA	2350	CB	LEU	566 566		73.1			890	89.64			1.04	•
ATOM ATOM	2351 2352	CG CD1	LEU	566		74.1			292	90.34			3.73	÷
ATOM	2353		LEU	566		72.6			299	90.15			1.29	š.
ATOM	2354	C	LEU	566		71.			418	87.26 87.31		.00 .00	6.69 6.50	₹ ÷
MOTA	2355	C	LEU	566 567		72.1			430	£7.40		.00	7.27	-
MOTA MOTA	2356 2357	N CA	CYS	567		69.			732	£7.65	8 1	.00 1	10.28	₹.
ATOM	2358	c	CYS	567		69.2			.013	69.12			13.50	:
ATOM	2359	0	CYS	567		69.			.113	69.98 66.70			13.64 12.07	÷
ATOM	2360	CB	CAE	567		60.			.017 .797	86.80			17.22	
MOTA	2361 2362	5G N	CYS ARG	567 568		69.			293	89.40			15.13	
MOTA MOTA	2363	CA	ARG	568		68.		38	. דרד	90.72			14.78	•
ATOM	2364	CB	ARG	568		68.			.310	90.79			17.37 20.45	÷
MOTA	2365	CC	ARG	568		70.	329		.829 .711	91.51 90.68			20.67	•
ATOM	2366 2367	CD NE	ARG ARG	568 568			045		.996				22.26	7
MOTA MOTA	2368		ARG	568			587		. 642	91.67			22.85	ž
ATOM	2369		1 ARG	568			531		.151				20.25	:
ATOM	2370		2 ARG	568			191		1.816 3.399				24.23 14.39	÷
ATOM	2371		ARG ARG	568 568			185 247		. 690				15.75	-
MOTA MOTA	2372 2373		LEU	569			046		7.752	92.2			11.39	
ATOM	2374		LEU	569			782		7.304			1.00	6.92 2.00	:
MOTA	2375			569			.005 .069		5.101 4.917			1.00	3.41	•
MOTA MOTA	2376		LEU 1 LEU	569 569			374		4.905			1.00	3.80	ŧ
ATOM	2378		2 LEU	569			. 852		2.67			1.00	2.00	
ATOM	237		LEU	569			.318		6.46			1.00	64 6.24	
ATOM	2380		LEU	569 570			.121 .015		9.221 8.64			1.00	9.65	
ATOM ATOM	2381 2381		HIS HIS	570			. 454		9.71		-		19.84	•
ATOM	238			570			. 841		0.81				11.04	
ATOM	238			570			.820		1.54° 2.49				10.31	
ATON	238		02 1115	570 570			. 845		1.42				14.50	
MOTA MOTA	238 238		DI HIS	570			.728		2.26		25		14.1	
MOTA			E2 HIS	570			. 28		2.92				12.65	
ATOM							.35		9.07 17.38			1.00	9.90 14.4	
ATOM		1 N					. 72		9.86			1.00		• -
MOTA MOTA			A GLN				. 65		9.36	97.0		1.00		
ATOM		13 C	B GLN	571			.18		88.80				11.4	
ATOM			S SLN).15).18		38.01	7 99. 12 100.		1.00) 13.3 21.5	3
ATOM			D GLN E1 SLN				1.16			37 101.			22.6	
ATOM ATOM			E2 SL:			5	9.11	.	38.90	62 101.	170	1.0	C 22.7	ó '
ATOM		98 3					9.71		40.50		308	1.0		
ATOM) SLN				D.09 8.44		41.5 40.1		285 419	1.0		
40TK 40TK			i ali Ca ali				7.34		41.0		658	1.0	0 5.:	2
ATO			CB AL	A 57	2	5	6.92	S.C.	41.7		356	0	(2.2	:7
ATO	1 24	03 -	AL.				6.21		40.2		195	1.0		
ATO: ATO:			D ALI				6.26 5.21		38.9		364	:.:		
ATO			CD PR				5.0		42.1	02 99.	602	1.5	ic 5.	15
ATO	M 24	07	CA PR	c 57	3		4.2		39.8		323	1.0		
ATO			CB PR				3.7			37 100. 99 100		1.0		
ATO ATO			CG PR C PR				3.0		39.7		. 377	1.0		
n.0						-		-						

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ATOM 2411 0 PRO 573 52.768 40.608 97.5	552 1.00 7.72 3
ATOM 2412 N THR 574 52.428 38.574 98.4	
ATOM 2413 CA THR 574 51.255 38.232 97.	
ATOM 2414 CB THP 574 51.075 36.738 97.	
ATOM 2415 OG1 THE 574 52.135 36.153 96.9 ATOM 2416 CG2 THR 574 49.712 36.324 97.5	
ATOM 2416 CG2 THR 574 49.712 36.324 97.1 ATOM 2417 C THR 574 50.119 38.852 98.1	
ATOM 2418 O THR 574 50.163 38.874 99.	
ATOM 2419 N ALA 575 49.087 39.324 97.1	
ATOM 2420 CA ALA 575 47.934 39.946 98.	
ATOM 2421 CB ALA 575 46.933 40.433 97, ATOM 2422 C ALA 575 47.282 38.960 99,	
ATOM 2422 C ALA 575 47.282 38.960 99.0 ATOM 2423 O ALA 575 46.480 39.355 100.	
ATOM 2424 N ARG 576 47.683 37.695 99.	
ATOM 2425 CA ARG 576 47.178 36.637 100.	
ATOM 2426 CB ARG 576 46.877 35.414 99.	
ATOM 2427 CG ARG 576 45.534 35.451 98. ATOM 2428 CD ARG 576 45.633 34.631 97.	
ATOM 2428 CD ARG 576 45.633 34.631 97.3 ATOM 2429 NE ARG 576 44.350 34.081 96.0	-
ATOM 2430 CZ ARG 576 44.171 33.438 95.	
ATOM 2431 NH1 ARG 576 45.188 33.261 94.8	
ATOM 2432 NH2 ARG 576 42.979 32.928 95.	
ATOM 2433 C ARG 576 48.090 26.216 101.	
ATOM 2434 O ARG 576 47.843 35.177 101. ATOM 2435 N GLY 577 49.167 36.963 101.	
ATOM 2435 N GLY 577 49.167 36.963 101. ATOM 2436 CA GLY 577 50.066 36.615 102.	
ATOM 2437 C GLY 577 51.201 35.638 102.	
ATOM 2438 O GLY 577 51.959 35.280 103.	
ATOM 2439 N ALA 578 51.263 35.140 161.	
ATOM 2440 CA ALA 578 52.332 34.245 100.	
ATOM 2441 CB ALA 578 51.842 32.360 99. ATOM 2442 C ALA 578 53.443 35.158 100.	
ATOM 2442 C ALA 578 53.443 35.158 100. ATOM 2443 0 ALA 578 53.278 36.384 100.	
ATOM 2444 N VAL 579 54.597 34.593 99.	
ATOM 2445 CA VAL 579 55.673 35.431 99.	
ATOM 2446 CB VAL 579 56.957 35.294 100.	247 1.00 9.32 6
ATOM 2447 CG1 VAL 579 56.734 35.863 101.	
ATOM 2448 CG2 VAL 579 57.363 33.860 100. ATOM 2449 C VAL 579 55.923 35.128 97.	
	939 1.00 9.09 6 452 1.00 8.40 5
ATOM 2451 N ARG 580 56.460 36.104 97.	
ATOM 2452 CA ARG 580 56.721 35.917 95.	
ATOM 2453 CB ARG 580 55.769 36.792 94.	
ATOM 2454 CG ARG 580 55.926 36.721 93. ATOM 2455 CD ARG 580 55.080 37.813 92.	503 1.00 7.88 6
	944 1.00 8.78 5 913 1.00 6.85 T
ATOM 2457 CZ ARG 580 52.719 38.362 93.	
ATOM 2458 NH1 ARG 580 53.050 39.581 93.	731 1.00 5.12 7
	466 1.00 2.00 7
	523 1.00 7.72 & 954 1.00 7.66 &
	954 1.00 7.66 8 827 1.00 6.07 7
	458 1.00 5.52 6
	803 1.00 4.84 6
	250 1.00 4.90 5
	045 1.00 3.60 4
	.822 1.00 5.69 6 .390 1.00 4.44 6
	390 1.00 4.44 5 165 1.00 5.88 5
ATOM 2470 CZ PHE 581 61.926 33.854 98.	944 1.00 3.43 5
	.944 1.00 3.43 6 .961 1.00 5.46 6
	.194 1.00 5.33 E
	.52500 6.16 ; .090 1.00 7.26 6
	.090 1.00 7.26 & .589 1.00 9.34 E
	.42300 10.74
	.280 :.00 11.49 😤
	.359 1.00 11.22 4
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	.530 1.06 14.19 4 .105 1.06 12.18 1
	.538 1.00 12.31
ATOM 2483 CZ3 TRF 582 61.001 42.247 90.	.356 1.00 11.65
	.617 1.00 16.33
	.429 1.00 7.94
	.041 1.00 5.37 E
	.334 1.90 9.15 4

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ATOM	2489	c i	CYS	583	6	3.15	4	38.449	E7.073			÷
ATOM			CYS	583		2.14		38.055	26.520			3
MOTA			CYS	583	6	4.50	7	36.591	ê7.876	1.00 11		÷
ATOM	2492		CYS	583	6	5.60		36.996	ē5.470	1.00 12		÷ 7
ATOM	2493	N	SER	584		3.89		39.453	66.606	1.00 11		÷
ATOM	2494	CA	SER	584		3.55		40.150	85.375	1.00 11		5
ATOM	2495	CB	SEP	584		53.21		41.612	£5.649	1.00 14		3
ATOM	2496	ЭG	SER	584		52.29		42.141	24.680 E4.531	2.00 11		Ę
MOTA	2497	•	SER	584		54.81		40.052	£4.990	1.00 14		,
MOTA	2498	Ĵ	SER	584		55.8		40.485 39.357	£3.390		3.82	7
MOTA	2499	N	LEU	585		64.74 65.81		39.214	€2.500		7.31	÷
MOTA	2500	CA	LEU	585		65.6		38.192	£1.374		5.24	÷
MOTA	2501	CB	LEU LEU	585 585		65.2		36.731	81.541		2.00	ē.
ATOM	2502	CS	LEU	585		65.9		35.888	80.486	1.00	2.00	÷
MOTA MOTA	2503 2504		LEU	585		65.6		36.271	82.912		5.67	5
ATOM	2505	5	LEU	585		66.1		40.562	81.832		8.79	5
ATOM	2506	õ	LEU	585		65.1	86	41.282	81.508		7.56	3
ATOM	2507	N	PRO	586		67.4	10	40.929	E1.637	1.00 1		7
ATOM	2508	CD	PRO	586		68.6		40.279	€2.160	1.00 1		6 5
MOTA	2509	CY	PRO	586		67.7		42.202	60.993	1.00 1		ń
MOTA	2510	CB	PRO	586		69.2		42.304	81.191	1.00 1		÷
MOTA	2511	CC	PRO	596		69.5		41.470	22.416 79.520	1.00 1		6
MOTA	2512	C	PRO	586		67.4		42.019	73.912	1.00 1		á
MOTA	2513	9	PRO	586		67.6	-	42.985	73.957	1.00 1		7
atom	2514	N	THR	587 587		66.6		42.949	77.569	1.00 1		Ê
MOTA	2515	CA	THR THF.	587		66.1		44.355	75.969			÷.
ATOM	2516	CB	THR	587		65.5		45.330	73.002			ŧ
MOTA	2517 2518		THR	587		65.0		44.408	75.929		7.05	6
MOTA MOTA	2519	C	THR	587		67.		42.186	75.657	1.00	2.00	6
MOTA	2520	ŏ	THF.	587		66.	739	41.308	75.948			9
ATOM	2521	N	ALA	588		68.	472	42.530	76.700			7
ATOM	2522	CA	ALA	588		69.	513	41.927	75.849		7.86	ó
ATOM	2523	CB	ALA	588		70.		42.342			8.95	é
ATOM	2524	C	ALA	588		69.		40.425			7.36	ó
ATOM	2525	0	ALA	588		69.		39.894			8.37 7.82	ā
MOTA	2526	N	ASP	589		68.		39.747			7.85	5
MOTA	2527	CA	ASP	589			745	38.300 37.684			5.24	ķ
MOTA	2528	CB	ASP	589			173 673	37.683			5.26	5
MOTA	2529	CG	ASP	589 589			088	38.045			6.3B	+
ATOM	2530		1 ASP 2 ASF	589			422	37.299			2.00	•
ATOM	2531 2532		ASF	539			341	37.84			7.96	:
MOTA ATOM	2533		ASP	589			080	36.65	75.38		7.86	5
MOTA	2534		THF.	590		66.	435	38.78			8.88	7
MOTA	2535		THF.	590		65.	040	38.45			10.02	÷
ATOM	2536		THP	590			118	39.57			8.46	÷
MOTA	2537) G	1 THF.	590			496				7.66	3
ATOM	2536	C C	2 THE	590			. 269					÷
ATOM	2539		THR	590			. 696				10.88	ė
ATOM			THF.	590			. 610				11.68	7
ATOM			SER	591			. 592 . 373				11.91	5
ATOM							. 692				13.98	÷
ATOM							.046		_		16.79	5
MOTA MOTA			SER				.405				11.64	:
ATOM		6 . 0				64	. 456	34.84			12.56	7
ATO							. 585					- 3
ATON			A SEP	. 592	!		. 60					
ATOM	254						.395					
4OTK	4 255	9 0					.79					
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ATO			i PHS B PHS				. 86					
ATO			B PHI G PHI				74					
ATO ATO			D1 PH				.04					
ATO			52 PH				3.39		62 (7.3	43 1.00		
ATO			E1 PH				.02		84 65.8			
ATO			E2 PH				9.38	_				
ATO			2 PH				9.68	6 35.2				
ATO		52 3	PH	E 59	3		3.84					
ATO	M 256	63 :	PE				4.30				11.09	
ATO			AV 3				4.22					
ATC			CA VA				5.28					
ATC	M 25	56 S	CF VA	1 59	4	Ó	6.58	96 30.4	09 71.3		. 7.1	•

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MOTA	2567		YAL	594		7.08		31.490	69.894	1.00	11.27	:
MOTA	2568		VAL	594		6.35		32.005	72.175	1.00	a.98	₹.
ATOM	2569	С	VAL	594		4.87		29.552	72.261	1.00	6.86	:
ATOM	2570	5	VAL	594		4.20		30.239	73.037	1.00	9.44	₹.
ATOM	2571	N	PRO	595		5.28		28.308	72.572	1.00	4.06	- 7
ATOM	2572	CD	PRO	595		5.91		27.414	71.592	1.00	4.50	•
ATOM	2573	CA	PRO	595		5.04		27.55B	73.802	1.00	4.33	4
ATOM	2574	CB	PRO	595·		5.62		26.185	73.468	1.00	4.07	•
ATOM	2575	CG	PRO	595		5.44		26.084	72.064	1.00	2.00	÷
ATOM	2576	C	PRO	595		5.72		28.142	75.048	1.30	3.58	
ATOM	2577	0	PRO	595		6.95		28.077	75.180	1.00	3.03	:
ATOM	2578	N C	LEU	596		4.92		28.692	75.955	1.00	3.21	
ATOM	2579	CA	LEU	596		5.42		29.282	77.199	1.00	4.16	:
ATOM	2580	C3	LEU	596		4.67		30.596	77.561	1.00	3.29	:
ATOM	2581 2582	CS	LEU LEU	596		5.38		31.870	78.068	1.00	2.00	•
ATOM	2583		LEU	596		4.50		32.639	79.002	1.00	3.47	÷
ATOM ATOM	2584	C	LEU	596 596		6.64 5.25		31.534 28.293	78.783	1.00	2.16	•
ATOM	2585	0	LEU	596		4.12		27.938	78.347 73.721	1.00	4.67	:
ATOM	2586	ĸ	GLU	597		6.38		27.861	78.900	1.00	2.52	÷ = -
ATOM	2587	CA	GLU	597		6.40		26.943	80.031	1.00	4.53 3.76	÷
ATOM	2588	СВ	GLU	597		7.56		25.980	79.909	1.00	2.00	•
ATOM	2589	CG	GLU	597		7.69		25.125	81.113	1.00	2.00	÷
ATOM	2590	CD	GLU	597		8.54		23.955	80.855	1.00	5.62	•
MOTA	2591		CLU	597		9.20		23.971	79.805		10.01	:
ATOM	2592	OE2	GLU	597		8.56		23.014	81.675	1.00	6.65	•
MOTA	2593	С	SLU	597		6.48		27.704	21.367	1.00	2.57	•
MOTA	2594	o	GLU	597		7.32		28.596	81.536	1.00	3.19	
MOTA	2595	N	LEU	598		5.59		27.358	82.296	1.00	3.03	:
MOTA	2596	CA	LEU	598	6	5.51	9	28.001	£3.600	1.00	2.16	÷
MOTA	2597	CB	LEU	598	6	4.15	59	28.670	83.777	1.00	2.00	÷
ATOM	2598	CG	LEU	598	6	3.75	6	29.657	82.681	1.00	2.00	÷
MOTA	2599	CD1	LEU	598	6	2.27	79	29.702	82.601	1.00	2.00	÷
MOTA	2600	CD2	LEU	598	6	4.36	58	31.027	82.888	1.00	2.00	÷
ATOM	2601	С	LEU	598	€	5.76	51	26.988	64.700	1.00	2.92	5
MOTA	2602	0	LEU	598	6	5.33	37	25.833	84.605	1.00	2.64	5
ATOM	2603	N	ARG	599	6	6.46	62	27.428	85.736	1.00	2.34	-
ATOM	2604	CA	ARG	599	€	6.80	04	26.580	86.862	1.00	3.62	
MOTA	2605	CB	ARG	599	€	8.25	54	26.115	86.710	1.00	6.78	į
ATOM	2606	CG	ARG	599	6	8.47	79	24.611	86.512	1.00	10.90	÷
MOTA	2607	CD	ARG	599		9.38		24.359	85.308	1.90	14.84	= =
ATOM	2608	NE	ARG	599		9.65		22.945	85.047		17.19	
atom	2609	CZ	APG	599		70.17		22.100	€5.942	1.90	17.80	•
ATOM	2610		AP.G	599		70.47		22.515	£7.182		17.23	-
ATOM	2611		ARG	599		0.45		20.845	E5.580		15.70	•
ATOM	2612	C	ARG	599		6.71		27.367	68.150	1.60	3.41	•
ATOM	2613	2	ARG	599		57.39		28.364	68.259	1.00	4.23	•
ATOM	2614	N	7XL	600		55.84		26.379	e9.081	1.20	2.87	
ATOM	2615	Ch	77.1	500		55.75		27.644	90.387	1.00	2.57	:
MOTA	2616	CB	7AL	600		54.32		28.001	90.825	1.00	2.02	:
ATOM	2617	CCI		600		54.33		28.512	\$2.248	1.36	2.00	•
ATOM	2618		VAL	600		53.73		29.035	89.917	1.00	2.30	÷
ATOM	2619	С	7AL	6 00		66.2		26.622	91.371	1.00	3.23	÷
ATOM	2620	0	7AL	600		65.74			91.426			:
ATOM	2621	N	THE	601		67.30		26.963	92.124	1.00	5.21	-
ATOM	2622	CÀ	THR	601		67. BI		25.043	93.098	1.00	6.74	÷
ATOM	2623	CB	THR	601		69.2		25.601	92.688	1.00	8.50	:
MOTA	2624	· 0G1		601		69.22 69.89		24.939	91.430		12.77	÷
ATOM	2625		THE	601		67.9		24.631 26.634	93.684	1.00	8.70	:
atom Atom	2626	2	IHR	601		68.2		27.822	94.481	1.00	8.74	
ATOM	2627	Ö	THR ALA	601 602		67.7		25.792	\$4.637 \$5.484	1.00	11.77	•
ATOM	2628 2629	CA		602		67.9		25.196	96.877	1.50	9.87	
ATOM	2630	CB	ALA ALA	602		67.2		25.191	97.745	1.00	3.62	:
ATOM	2631	5	ALA	602		69.4		26.180	97.153		3.55	:
ATOM	2632	Ö	hih	602		70.1		25.324	96.613	1.33		:
ATOM	2633	N.		603		69.8		27.969	93.036		11.56	-
ATOM	2634	CA	hih hih	503		71.2		27.162	98.415	1.23	9.78 7.23	:
ATOM	2635	CB	hih	603		71.5		28.370	99.300	1.11	5.77	
ATOM	2636	5	ALA	603		71.B		25.882	99.070	1.33	5.23	:
ATOM	2637	Š	ALA	503		73.0		25.785	9.320		4.90	:
ATOM	2638	N	SER	604		71.0		24.892	99.324	1.23	5.87	-
ATOM	2639	CA	SER.	604		71.4		23.639	99.897		7.44	:
ATOM	2640	CB	SER	604		70.4			100.740	: . : :	5.37	:
MOTA	2641	OG	SER	604		69.7		22.024	\$9.997		5. 42	:
MOTA	2642	c	SER	604		71.9		22.689	98.777	1.2	9.18	:
ATOM	2643	•	SER	604		72.4		21.617	93.042	1.0	11.68	
ATOM	2644	N	STX	605		71.6		23.070	\$7.535	1.1		

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ATOM	2645	CA	GLY	605	71.94	4 2	22.262	96.378		.17	:
ATOM	2646		GLY	605	70.70	9 2	21.620	95.785		.43	:
ATOM	2647	٥	GLY	605	70.71		21.198	94.631	_	.81	-
ATOM	2648		ALA	606	69.63		21.606	96.573		.11	:
MOTA	2649		ALA	606	68.37	-	21.001	96.194		. 20	
MOTA	2650		ALA	606	67.49		20.885 21.770	97.387 95.113		.88	
MOTA	2651		ALA	606	67.66 67.45		22.974	95.234		.80	÷
ATOM	2652	o N	ALA PRO	606° 607	67.2		21.063	94.074	-	5.21	•
ATOM	2653 2654	CD	PRO	607	67.4		19.636	93.821		5.78	÷
atom Atom	2655	CA	PRO	607	66.5		21.660	92.950		7.75	•
ATOM	2656	CB	PRO	607	66.6		20.587	91.845		7.27	-
ATOM	2657	ÇG	PRO	607	67.6		19.620	92.355		5.40 5.86	₹ :
MOTA	2658	5	PRO	607	65.0		21.969 21.084	93.220 93.599		6.25	
ATOM	2659	0	PRO	607 608	64.2 64.6		23.215	92.953	-	6.55	:
MOTA	2660	N CA	ARG ARG	608	63.2		23.658	93.095		6.82	•
MOTA MOTA	2661 2662	CB	ARG	608	63.1		25.105	93.591		7.55	•
MOTA	2663	CG	ARG	608	63.5		25.320	95.066	1.00 1		:
ATOM	2664	CD	ARG	608	62.6	80	24.474	95.992	1.00 1		•
MOTA	2665	NE	ARG	608	61.1		24.719	95.820	1.00 1		÷
ATOM	2666	CZ	ARG	608	60.5		25.828	96.200	1.00 1		-
MOTA	2667		ARG	608	61.1		26.817	96.773 96.048	1.00 1		-
MOTA	2668		ARG	608	59.2 62.5		25.936 23.548	91.739	1.00	6.91	:
MOTA	2669	C	ARG ARG	608 608	£1.6		22.836	91.612	1.00	8.99	:
MOTA MOTA	2670 2671	9	TYP.	609	63.0		24.194	90.700	1.00	7.03	-
ATOM	2672	CA	TYP.	609	62.4		24.140	89.406	1.00	7.82	•
MOTA	2673	CB	TYP	609	61.5	332	25.394	89.203	1.00	9.92	:
ATOM	2674	ÇG	TYR	609	60.		25.684	90.298	1.00 1		•
MOTA	2675		TYP	609	60.		26.798	91.137	1.00		•
MOTA	2676		TYR	609	59.		27.078 24.852	92.156 90. 49 9	1.00		•
MOTA	2677		TYP	609 609	59.4 58.4		25.120	91.506	1.00		:
ATOM	2678 2679	CE2	TYR TYR	609	58.		26.235	92.326	1.00		₹.
MOTA MOTA	2680	ОН	TYP	609	57.		26.529	93.255	1.00	17.36	:
ATOM	2681	Ç	TYP.	609	63.	316	24.032	88.193	1.00	7.45	•
ATOM	2682	0	TYR	609	64.		24.514	88.207	1.00		:
MOTA	2683	N	HIS	610	€2.		23.416	87.137	1.00	4.17	÷
ATOM	2684		HIS	610		536	23.308	85.886 85.775	1.00	3.51 2.85	:
ATOM	2685		HIS	610		306	21.995	84.524	1.00	2.00	;
ATOM	2686		HIS 2 HIS	610 610		112 692	22.830		1.00	2.00	4
MOTA MOTA	2687 2688		1 HIS	610		346	20.681	83.896	1.00	2.00	-
MOTA	2689		1 HIS	610		030	20.893	62.786	1.00	2.00	•
ATOM	2690		2 HIS	610		250	22.189			2.00	•
ATOM	2691		HIS	610		500	23.456	84.774		3.94	:
MOTA	2692		HIS	610		459	22.824			4.37	-
MOTA	2693		ARG	611		790 858	24.306 24.561			2.00	
ATOM	2694			611 611		946	25.70			2.00	4
MOTA MOTA	2693 2690			611		476	25.57			5.34	:
ATOM	269			611		.701	25.89		1.00	2.76	
ATOM	269			611		. 501	26.83			4.99	
ATOM	269			611		. 647	27.83			4.31	
ATOM	270		11 ARG	611		.850 .605				9.07 2.00	
ATOM			12 ARG	611		. 657				2.00	
ATOM	270	2 · C	ARG ARG	611 611		.800				3.11	
MOTA MOTA						.074				2.76	
ATOM						. 669		6 79.11			
ATOM					2 63	. 056					
ATOM	270		G1 VAL			. BO					
ATOM			G2 VAL		-	. 917					
ATOM					-	.490 .382					
ATOM						. 674					
ATOM ATOM					-	.55					
ATON			B ILE			.88		3 78.27	0 1.00	2.00	
ATOM			G2 ILE		3 59	9.24	28.2				
ATO	1 27	15 C	G1 ILE	61	3 60	0.89					
ATO			D1 ILE			0.26					
ATOTA						0.99 2.16					
OTA OTA						2.16 0.01				3.3	
OTA			A HI			0.25			11 1.00	4.6	3
ATO			B H1		.4 5	9.60	4 29.4	27 72.9	7001	2.3	
ATO			CC HI	5 61	.4 ć	(1.44	7 28.4	10 72.2	71 1.00	0 2.10	U

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ATOM	2723	CD2	HIS	614	61.35	3	28.536	71.281	1.00	2.96	÷
ATOM	2724	ND1	HIS	614	60.44		27.075	72.609	1.00	4.63	i
MOTA	2725		HI5	614	61.31		26.419	71.865	1.00	2.00	÷
ATOM	2726		HIS	614	61.87		27.284	71.051	1.00	6.31	7
ATOM	2727	٥ ن	HIS	614	59.58		31.311	74.664	1.00	3.58	ક
ATOM ATOM	2728 2729	N.	HIS ILE	614 615	58.41 60.31	_	31.306	75.046	1.00	2.50	3
ATOM	2730	CA	ILE	615	59.71	_	32.412 33.661	74.674	1.00	2.76	7
ATOM	2731	CB	ILE	615	60.77		34.768	75.108 75.221	1.00	2.55	÷
ATOM	2732		ILE	615	60.10		36.115	75.507	1.00	2.49 2.99	÷
MOTA	2733	CG1	ILE	615	61.78		34.387	76.307	1.00	2.00	6
MOTA	2734	CD1	ILE	615	63.06	7 .	35.246	76.351	1.00	2.00	÷
MOTA	2735	C	ILE	615	58.56		34.079	74.205	1.00	3.27	÷
ATOM	2736	0	ILE	615	57.60		34.687	74.651	1.00	5.04	.3
ATOM ATOM	2737 2738	N CA	asn Asn	616 616	58.63 57.61		33.673	72.943	1.00	5.73	7
ATOM	2739	CB	ASN	616	58.20		34.015 33.893	71.945 70.513	1.00	4.76	÷
ATOM	2740	CG	ASN	616	58.86		32.539	70.236	1.00	2.00 2.00	6 6
MOTA	2741	OD1	ASN	616	58.41		31.767	69.399	1.00	2.00	3
MOTA	2742		ASN	616	59.95		32.273	70.910	1.00	2.00	Ź
ATOM	2743	c	ASN	616	56.28		33.247	72.124	1.00	4.60	6
atom atom	2744 2745	И О	ASN	616	55.26	_	33.632	71.581	1.00	6.70	3
ATOM	2746	CA	GLU	617 617	56.28 55.08	_	32.240	72.989	1.00	4.63	7
ATOM	2747	CB	GLU	617	55.42		31.444 29.951	73.242 73.185	1.00	5.16	÷
ATOM	2748	CG	GLU	617	56.38		29.633	72.086	1.00	4.92	é
ATOM	2749	CD	GLU	617	56.43		28.180	71.704		8.53 11.83	÷
ATOM	2750	CE1	GLU	617	56.65		27.922	70.498		15.40	
ATOM	2751	JE2	CLU	617	56.27		27.297	72.575		14.68	ā
ATOM	2752	C	GLU	617	54.43		31.744	74.587	1.00	4.18	÷
ATOM	2753 2754	S	GLU	617	53.44		31.127	74.930	1.00	7.74	a
ATOM ATOM	2755	N Ca	VAL VAL	618 618	54.99 54.43		32.667	75.354	1.00	3.63	7
ATOM	2756	CB	VAL	618	55.36		32.98B 32.566	76.655 77.870	1.00	2.00	6
ATOM	2757	CG1		618	55.66		31.109	77.838	1.00	2.00 2.00	6 6
ATOM	2758	CG2	VAL	618	56.65		33.337	77.890	1.00	2.00	6
ATOM	2759	С	VAL	618	54.11	9	34.459	76.727	1.00	2.00	6
MOTA	2760	e	VAL	618	54.60		35.167	77.616	1.00	2.77	â
atom Atom	2761 2762	.N	VAL	619	53.33		34.937	75.778	1.00	2.00	7
ATOM	2763	CA CB	VAL VAL	619 619	52.97 52.76		36.345	75.792	1.00	3.10	6
ATOM	2764	CG1		619	52.74		36.886 38.409	74.407	1.00	2.32	5
ATOM	2765		VAL	619	53.88		36.412	73.519	1.00	2.43 7.61	5 6
MOTA	2766	ε	VAL	519	51.70		36.587	76.589	1.00	4.11	÷
ATOM	2767	0	VAL	619	50.81		35.731	76.610	1.00	6.41	3
MOTA	2768	N	LEU	620	51.63		37.734	77.268	1.00	2.53	7
ATOM ATOM	2769 2770	CA CB	LEU LEU	620	50.49 50.70		28.143	78.080	1.00	3.37	÷
ATOM	2771	CG	LEU	620 620	49.61		37.790 37.183	79.554	1.00	3.39	÷
ATOM	2772		LEU	520	50.23		37.163	80.438 81.775	1.00	3.95	6
ATOM	2773		LEU	620	48.30		37.985	80.529	1.00	5.62 3.31	÷
ATOM	2774	C	LEU	620	50.38		39.654	77.920	1.00	5.44	÷
atom	2775	٥	LEU	620	50.85		40.437	78.736	1.00	7.07	ā
ATOM	2776	N	LEU	621	49.73		40.044	76.834	1.00		7
ATOM ATOM	2777 2778	CA CB	LEU	621	49.54		41.432	76.465	1.00	5.70	5
ATOM	2779	CS	LEU LEU	621 621	48.83 19.46		41.498	75.111	1.00	5.58	÷
ATOM	2780			621	48.39		40.971 40.832	73.845	1.00	2.00	÷
ATOM	2781		LEU	621	50.54		41.903	73.377	1.00	2.42	ó
MOTA	2782	2	LEU	621	48.73		42.253	77.427	1.00		÷
ATOM	2783	5	LEU	621	47.94		41.728	78.198	1.00	8.04	3
ATOM	2784	2.	ASP	622	48.92		43.565	77.355		11.43	7
ATOM	2785 2786	CA	ASF	622	48.14		44.513	78.128		10.55	÷
atom atom	2787	CB	ASP ASP	622 622	48.67 49.74		45.938	77.968	1.00		á
ATOM	2788		ASF	622	50.39		46.300 47.342	78.963 78.724		11.16	:
ATOH	2789		ASF	622	49.92		45.580	79.976		12.42	; ;
ATOM	2790	2	ASF	622	46.85		44.429	77.336		10.98	•
ATOM	2791	5	ASP	622	46.80	67	44.075	76.152		11.16	.3
ATOM:	2792	3	ALA	623	45.75		44.808	77.965	7.00	13.11	?
ATOM	2793	SY	ALA	623	44.45		44.764	77.326	1.00	12.49	÷
MOTA MOTA	2794 2795	3 2	ala Ala	623	43.3		44.723	78.402		13.24	3
ATOM	2796	3	ALA	623 523	44.20 45.03		45.975	76.399		10.77	•
ATOM	2797	š	PRO	624	43.3		46.953 45.890	76.489 75.462	1.00	11.45	.3 7
ATCM	2798	CD	PRC	624	42.6		44.628	75.175	1.00		,
MOTA	2799	CA	PPC	624	42.9		46.928	74.486	20		4
ATOM	2800	CB	PP.C	624	41.9	33	46.241	73.632	00		.,

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ATOM	2801	CG	PRO	624		42.33		44.75		3.736 5.095	1.00	9.99		
ATOM	2802	C	PRO	624		42.3		48.19	-	6.05E	1.00		o =	
MOTA	2803	၁	PRO	624		41.59		48.13 49.35		4.518	1.00		_	
ATOM	2804	N	VAL	625 625		42.1		50.63		4.969	1.00	8.5	7 5	
ATOM	2805	CA	VAL VAL	625		43.2		51.67	_	5.160	1.00	8.1		
MOTA	2B06	CB	VAL	625		44.0		51.32		6.386	1.00	10.:		
ATOM	2807 2808		VAL	625		44.1		51.74		3.933	1.00	6.4		
MOTA MOTA	2809	c	VAL	625		41.1	36	51.19		3.950	1.00	11.0	9 3	
ATOM	2810	.5	VAL	625		40.7		50.51		2.970		11.3	_	
ATOM	2811	N	GLY	626		40.6		52.39	-	4.243		10.5	_	
ATOM	2812	Ch	GLY	626		39.6		53.09		3.389 12.843		14.1		
MOTA	2813	C	GLY	626		38.3		52.4		11.775		14.3		•
ATOM	2814	2	GLY	626		37.9 37.8		52.9		3.565		16.0	6	:
ATOM	2815	N	LEU	627 627		36.5		50.8	_	73.112		17.5	3	£
MOTA	2816	CA	LEU	627		36.1		49.7		74.092	1.00	13.8		É
MOTA	2817 2818	CG	LEU	627		34.9		48.9		73.631		13.2		÷
MOTA MOTA	2819		LEU			35.3	199	48.1		72.467		15.		5
ATOM	2820		LEU			34.4		48.0		74.740		12.		6 5
ATOM	2821	Ç	LEU	627		35.4		51.6		72.928		18.		3
ATOM	2822	0	LEU			35.		52.5		73.881 71.682		17.		7
ATOM	2823	N	VAL			34.		52.8		71.355		19.		÷
MOTA	2824	CA	VAL			33.1 34.		54.1		70.490		18.		÷
MOTA	2825	CB	VAL			34.		55.1		71.318		19.		é
ATOM	2826		1 VAI 2 VAI			34.		53.7		69.244		18.		÷
MOTA MOTA	2827 2828		VAI			32.		52.0		70.609		21.		÷
ATOM	2829		VAI			33.	146	51.1		69.743		0 19.		9 7
ATOM	2830		ALI	62	9		528	52.		71.036		0 21.		5
ATOM	2831	CA					393	51.		70.440		0 21. 0 25.		6
ATOM	2832						532	50.5 52.		69.664	_	0 22.		÷
ATOM	2833		AL				593 684	53.		69.980		0 23.		8
MOTA	2834		AL	_			823	52.		68.659	_	0 22.		7
ATOM	2835		AR AR				014	52.		67.845		O 19.	. 90	÷
MOTA	2836 283						873		703	66.809		0 19		ő
MOTA MOTA	283						.087		154	67.175		0 22		5
ATOM	283					29	. 565		016	65.999		0 24		5 7
MOTA	284						. 366		461	66.223		0 26 0 28		5
MOTA	284						. 627		112	67.368 68.45		0 26		7
ATOM	284		11 AP				.108 .421		460	67.42		00 25		7
ATOM	284	-	H2 AF				.867		308	67.12		00 13		÷
ATOM	284 284		A.		0		. 945		. 133	66.74		00 19		3
MOTA MOTA	284				31	25	.787	53.	.049	66.94		00 18		7
ATOM	284				31		. 650		.498	66.23		30 18		ē ē
ATOM	284				31.		.379		.267	66.60		00 18 00 17		5
ATOM	284				31		. 269		.408	67.21 66.71		00 1E		5
MOTA			D1 L	_	31		. 275		.967 .322	68.74		00 18		÷
MOTA		-	D2 L	_	31		2.351 1.820		.770	64.79	-	00 21		5
ATOM					31 31		.73		.915	64.34		00 2		а
ATOM					32		5.09		.758	64.05	7 1.	00 2		7
ATOM NOTA					32		5.17		. 975			00 2		÷
ATOM					32		5.60		. 699			00 2		÷
ATON				LA 6	32		3.77		.420			00 2		÷ 8
ATON		58 ' 3			32		2.96		. 604			00 2		7
ATO					33	_	3.54 2.23		3.700 1. 36 6			00 9		÷
ATO			-		533 533		2.23 2.43		5.880			00 9		÷
ATO					632		2.35		6.775		13 1	.00 9	0.30	÷
ATO: ATO:			נסכ גסכ		633		1.77		6.363		47 1	.00 9		.3
ATO	-		OD2 1		633		2.85	2 5	7.977			.00 9		3
ATO					€33		1.46		3.894			.00 9		
ATO		66	2 1	ASP	633		0.2		3.666			.00 9		3
ATO					634		2.13		3.74				21.30	
ATO		68			634		21.42 22.3		3.465 3.75				06.30	
ATO				GLU GLU	634 634		22.B		5.20				90.20	•:
OTA OTA		970 371		GLU	634		23.7		5.52		5: 1	.00	9¢.00	
ATO		372	DE1		634	:	24.0	12 5	4.62		£: :	.co	90.20	3
ATC		373	JE2		634		24.2		5.69				90.00	:1
ATC	2H 2	874		CTO	634		20.9		2.02				90.30	
ATC		875		CLU	634		20.0		1.72				90.00 90.00	
ATO		876	2	SER	635		21.4 21.0		51.13 49.72				90.00	
ATC		877	CA CB	ser Ser	635 635		21.0 22.2		48.82				90.00	
TA	un 2	878	-0											

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ATOM	2879	OG	SER	635	23.189	49.037	60.063	1.00 90.00 3
ATOM	2880	С	SER	635	20.328	49.370	60.435	1.00 90.00 5
ATOM	2881	0	SER	635	19.394	48.552	60.427	1.00 90.00 3
ATOM	2882	N	GLY	636	20.780	50.010	61.488	1.00 90.00 7
ATOM ATOM	2883 2884	CA C	GLY	636	20.217	49.834	62.821	1.00 90.00 \$
ATOM	2885	o	GLY	636 636	20.996 20.541	48.771	63.586	1.00 90.00 5
ATOM	2886	N	HIS	637	22.203	47.640 49.107	63.790 64.010	1.00 90.00 £ 1.00 29.39 7
ATOM	2887	CA	RIS	637	22.920	48.155	64.847	1.00 28.30 5
ATOM	2888	CB	RIS	637	23.190	46.817	64.148	1.00 27.49 5
MOTA	2889	CG	HIS	637	23.915	46.854	62.796	1.00 26.32 5
atom Atom	2890 2891		HIS HIS	637 637	25.124	47.337	62.400	1.00 26.14 5
ATOM	2892			637	23.338 24.176	46.289 46.428	61.665	1.00 26.56 7
ATOM	2893		HIS	637	25.247	47.050	61.079	1.00 26.93 6 1.00 26.35 7
ATOM	2894	С	HIS	637	24.223	48.651	65.427	1.00 27.39 6
MOTA	2895	0	HIS	637	24.505	49.862	65.452	1.00 27.46 3
atom Atom	2896 2897	N CA	VAL	638	24.921	47.631	65.868	1.00 25.98 7
ATOM	2898	CB	VAL	638 638	26.119 26.169	47.770	66.646	1.00 22.67 5
ATOM	2899		VAL	638	26.966	46.693 47.127	67.730 68.963	1.00 23.93 5 1.00 24.68 5
ATOM	2900	CG2	VAL	638	24.781	46.310	68.251	1.00 23.20 5
ATOM	2901	C	VAL	638	27.422	47.694	65.877	1.00 21.16 5
ATOM	2902	0	VAL	638	27.763	46.687	65.236	1.00 17.80 3
atom atom	2903 2904	N	VAL	639	28.129	48.808	65.940	1.00 19.71 7
ATOM	2905	CA CB	VAL VAL	639 639	29.417 29.362	48.927	65.309	1.00 21.49 5
ATOM	2906		VAL	639	30.383	49.967 51.140	64.127 64.296	1.00 22.97 5 1.00 22.32 5
MOTA	2907			639	29.531	49.189	62.796	1.00 21.09 4
MOTA	2908	C	VAL	639	30.503	49.131	66.402	1.00 18.72 6
ATOM	2909	0	VAL	639	30.569	50.164	67.103	1.00 15.61 3
atom Atom	2910 2911	N CA	LEU	640	31.245	48.035	66.588	1.00 17.29 7
ATOM	2912	CB	LEU	640 640	32.312 32.296	47.853 46.385	67.567	1.00 15.07 6
ATOM	2913	CG	LEU	640	31.948	45.925	68.002 69.398	1.00 11.06 5 1.00 9.33 6
ATOM	2914	CD1	LEU	64 D	30.755	46.635	69.940	1.00 6.96 5
ATOM	2915		LEU	640	31.703	44.456	69.328	1.00 7.60 5
ATOM	2916	C	LEU	640	33.727	48.158	67.106	1.00 15.19 6
atom atom	2917 2918	N O	LEU ARG	640 641	34.319	47.345	66.393	1.00 13.52
ATOM	2919	CA	ARG	641	34.320 35.717	49.236 49.564	67.616 67.269	1.00 16.40 7 1.00 18.02 6
ATOM	2920	CB	ARG	641	35.744	50.820	66.406	1.00 18.02 5
ATOM	2921	CG	ARG	641	36.505	50.60B	65.100	1.00 23.80 5
ATOM	2922	CD	ARG	641	35.742	51.114	63.884	1.00 25.92 6
atom atom	2923 2924	NE CZ	ARG	641	34.649	50.212	63.502	1.00 26.12 7
ATOM	2925	NH1	ARG	641 641	33.446 33.173	50.620 51.935	63.025 63.013	1.00 27.21 £
ATOM	2926		ARG	641	32.538	49.716	62.685	1.00 24.02 T
MOTA	2927	С	ARG	641	36.638	49.707	68.527	1.00 17.87 6
ATOM	2928	9	ARG	641	36.119	49.879	69.655	1.00 19.51 3
atom atom	2929 2930	N ÇA	TRP	642	37.972	49.598	68.366	1.00 16.84
ATOM	2931	CB	TRP TRP	642 642	38.925 38.765	49.723 48.534	69.515 70.453	1.00 14.61 5
ATOM	2932	CG	TRP	642	39.106	47.243	63.819	1.00 13.71 5 1.00 9.75 5
ATOM	2933		TRP	642	38.203	46.359	69.133	1.00 10.16 #
ATOM	2934		TP.P	642	38.926	45.195	68.814	1.00 10.08 #
ATOM ATOM	2935 2936		TP.P	642 642	36.855 40.304	46.438	68.760	1.00 8.27 5
ATOM	2937		TRP	642	40.208	46.612 45.37?	69.860 69.267	1.00 7.42 ÷ 1.00 10.16 ÷
ATOM	2938		TPP	642	38.345	44.116	68.150	1.00 8.53
ATOM	2939		TRP	642	36.289	45.374	68.098	1.00 7.26 5
ATOM	2940		TRF	642	37.035	44.225	67.803	1.00 7.13 6
MOTA MOTA	2941 2942	C O	TP.F TP.P	642 642	40.424	49.824	69.178	1.00 15.14
ATOM	2743	N	LEU	643	40.79E 41.275	49.704 49.382	68.006 70.207	1.00 17.51 E
ATOM	2944	CA	LEU	643	42.747	50.063	70.039	1.00 12.07
ATOM	2945	CB	LET	643	43.310	51.312	70.676	1.00 9.27 ÷
MOTA	2946	CG	LET	643	42.887	52.62?	70.081	1.00 9.05
atom Atom	2947 2948		LET	643	43.784	53.715	70.583	1.00 7.00 5
ATOM	2948	502	LEU Leu	643 643	43.012 43.508	52.525 48.891	68.601 70.662	1.00 9.98
ATOM	2950	5	LEU	643	43.096	48.351	71.697	1.00 15.42 6
ATOM	2951	N	PRO	644	44.645	48.493	70.059	1.00 15.99
ATOM ATOM	2952	CD	PPC	644	45.206	49.056	68.817	1.00 15.21 5
ATOM	2953 2954	CA CB	PRC PRC	-644 644	45.481 46.485	47.381 47.175	70.556	1.00 14.66
ATOM	2955	CG	PRC	644	46.642	48.573	69.412 69.867	1.00 15.17
MOTA	2956	C	PPC	644	46.192	47.793	71.851	1.00 11.57

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ATOM	2957	٥	PRO	644	4	6.14		.978	72.209		0 12.3		
ATOM	2958	N	PRO	645		6.80		. 824	72.588		0 10.6		
ATOM	2959	CD	PRO	645		6.83		3.392	72.229		00 10.4 00 9.5		
MOTA	2960	CA	PRO	645		7.53		7.049	73.851		00 10.2		
ATOM	2961	CB	PRO	645		8.27		3.746 8.742	73.502				
MOTA	2962	CG	PRO	645		17.32 18.47	_	8.178	73.572				
ATOM	2963	C	PRO	645		9.21	-	B.142	72.60		00 11.	71 3	,
MOTA	2964	0	PRO	645		8.43		9.229	74.37			63	•
atom	2965	N	PRO	646 646		47.68		9.431	75.618			62 😚	•
MOTA	2966	CD	PRO	646		49.33		0.350	74.10		00 9.	90 -	5
MOTA	2967	CA	PRO PRO	646		49.00	4 5	1.345	75.21	7 1.	00 9.		5
MOTA	2968 2969	CG	PRO	646		47.61		0.941	75.67		00 11.		6
MOTA MOTA	2970	Č	PRO	646		50.80	9 4	9.956	74.11		00 13.		
MOTA	2971	ŏ	PRO	646		51.20		8.918	74.67		00 14.		5 7
ATOM	2972	N	GLU	647		51.6		0.786	73.47		00 13.		÷
ATOM	2973	CA	GLU	647		53.0		0.546	73.38 74.55		00 15.		5
ATOM	2974	CB	GLU	647		53.7		1.217	74.38		00 19.		÷
ATOM	2975	CG	GLU	647		53.7	_	3.470	75.64		00 20.		6
ATOM	2976		GLU	647		53.6		33.215	76.71		.00 22		ŝ
ATOM	2977		CLU	647 647		55.1		54.305	75.56		.00 19		ŧ
MOTA	2978		GLU	647		53.4		19.082	73.21		.00 14	.37	Ş
MOTA	2979		GLU	647		54.5		48.697	73.79	5 1	.00 18	.36	•
ATOM	2980		THR	648		52.7		48.316	72.38	1 1	.00 11		7
MOTA	2981		THE	64B		53.0		46.899		52 1		.00	÷
ATOM	2982 2983		THR	648		51.8		45.984	72.4			.78	÷
MOTA MOTA	2984		1 THR	648		51.5	52	46.119			.00 10		ē
ATOM	2985		2 THR	648		52.1		44.533				.04	÷
MOTA	2986		THR	648		53.2		46.761				.27	é 3
ATOM	2987		THR	648		52.		47.370				.52 .20	ה ר
ATOM	2988	e N	PRO	649		54.3		45.968				.54	ę.
MOTA	2989			649		55.		45.245				.88	5
ATOM	299			649		54.		45.49				.46	6
MOTA	299			649		56.3 56.3		44.592				.39	6
atom	299					53.		44.70				1.17	6
MOTA	299		PRO			52.		44.10				.10	â
ATOM	299		PRO			54.		44.40				0.01	7
ATOM	299		MET MET				645	43.36			1.00	3.79	÷
ATOM	299 299						158	41.96		70		8.66	÷
MOTA MOTA	299					55.	676	41.83				7.85	
ATOM						56.	219	41.81				7.28	15
ATOM					Ó	56.	577	40.14				2.00	ş
ATOM			MET	65	0		112	43.35			1.00 1		
ATOM		2 0	ME				478	42.28			1.00 1		3
ATOM							.581	44.54			1.00 1		÷
MOTA	300						.136	44.80			1.00 1		•
ATOM			B TH				.858 .419	47.19		162	1.00 1		į
ATOM			G1 TH				.364	46.50		187	1.00 1		ř
ATOM			G2 TH				.353	43.70		039	1.00 1		5
ATOM							309	43.20	64 65.	454	1.00 1	6.75	3
ATO							.866	43.4	78 63.	829	1.00 1		
ato: Ato:			A SE			49	.110	42.6	23 62.	863	1.00	6.89	÷
ATO			B SE				.510	42.9		416	1.00	5.16	÷
ATO			G SE	R 6:			.405	41.9		895	1.00	4.04	:
ATO		14 .			52		. 235	41.1		151	1.00	9.34	ž
ATO	M 30		O SE		52).034).523	40.2 40.7		.274 .390	1.00	7.77	5
ATO			N H		53).584			B 05	1.00	6.49	ž.
ATO		•-	CA B		53		.991			. 253	1.00	6.61	÷
ATO			CB H		53 53		.892			.029	1.00	9.79	•
λTO					53		2.285			.288	1.00	9.28	÷
ATO			CD2 H: ND1 H:		53 53		2.471			.438		10.33	
otk Otk			CE1 H		53		3.171		68 62	. 395	1.00	5.42	÷
ATO ATO			NE2 H		53	5	3.071			. 291	1.00	7.91	•
ATC					53		8.476			.830	1.00	4.62	:
ATC		025			53		7.989			.994	1.00	5.90	3
λTC		026		LE S	54		8.04			.470	1.00	5.11	
ATC		027	CA I	LE 🤄	54		7.07		145 67	.580	1.00	4.75	
ATC	DM 3	028			554		7.05			.355 9.653	1.00	5.93	
λTC		029	CG2 I		554		6.25			3.760	1.00	3.24	
ATC		030	CG1 I	_	554		8.46			.131	1.00	2.00	
ATO		031	CD1 I		654 654		5.63			7.156	1.00	5.10	
ATO		032			654		4.98			5.395		7.39	
TA TK		1033 1034			655		5.21	-		7.7:3		5.70	
AT	- ·		,			7							

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MOTA	3035	CA	ARG	655	43.8	56	38.107	67.582	1.00 4.70	5
ATOM	3036	CB	ARG	655	43.9	47	36.60B	67.851	1.00 6.54	6
ATOM	3037	CG	ARG	655	42.7		35.835	67.393	1.00 12.78	5
MOTA	3038	CD	ARG	655	42.9		35.234	66.013	1.00 19.16	5
MOTA	3039	NE	ARG	655	41.6		35.243	65.243	1.00 25.22	7
ATOM	3040	CZ	ARG	655	41.4		34.509	64.155	1.00 28.18	5
ATOM	3041		ARG	655	42.4		33.699	63.683	1.00 29.93	7
ATOM	3042		ARG	655	40.3		34.523	63.465	1.00 30.11	7
atom atom	3043 3044	0	ARG ARG	655 655	43.0 43.5		38.786	68.687	1.00 4.93	6
ATOM	3045	N	TYR	656	41.7		39.225 38.916	69.706	1.00 4.78	9
ATOM	3045	CA	TYR	656	40.B		39.533	68.485 69.491	1.00 3.05 1.00 4.57	7
ATOM	3047	CB	TYR	656	40.3		40.886	69.041	1.00 5.74	6
ATOM	3048	CG	TYR	656	41.3		41.973	69.131	1.00 11.08	5
ATOM	3049	CD1	TYP.	656	41.9		42.423	67.995	1.00 11.86	6
ATOM	3050	CE1	TYR	656	43.0	29	43.341	68.077	1.00 13.79	6
ATOM	3051	CD2	TYR	656	41.7		42.482	70.366	1.00 13.83	6
MOTA	3052	CE2	TYR	656	42.7		43.407	70.461	1.00 14.75	6
MOTA	3053	CZ	TYR	656	43.4		43.B26	69.307	1.00 14.26	6
MOTA	3054	OH	TYR	656	44.4		44.701	69.373	1.00 19.33	8
MOTA MOTA	3055 3056	0	TYR TYP	656 656	39.6 39.5		38.646	69.848	1.00 7.31	5
ATOM	3057	N	GLU	657	38.9		37.608 39.048	69.210 70.905	1.00 7.58	8 7
ATOM	3058	CA	GLU	657	37.7		38.359	71.431	1.00 9.63 1.00 9.06	, 6
ATOM	3059	СВ	GLU	657	38.1		37.385	72.555	1.00 11.39	6
ATOM	3060	CG	GLU	657	36.8		36.766	73.217	1.00 14.76	6
ATOM	3061	CD	GLU	657	36.7		35.254	72.977	1.00 17.29	6
ATOM	3062	GE1	GLU	657	36.1	.57	34.838	71.945	1.00 19.32	ē
ATOM	3063	QE2	CLU	657	37.2		34.472	73.826	1.00 18.57	8
ATOM	3064	C	GLU	657	36.8		39.366	72.006	1.00 10.04	6
ATOM	3065	0	GLU	657	37.1		40.033	72.985	1.00 8.78	8
ATOM	3066	N	VAL	658	35.6		39.428	71.412	1.00 13.32	7
atom atom	3067 3068	CA CB	VAL VAL	658 658	34.5 33.6		40.334	71.819	1.00 15.04	6
MOTA	3069		VAL	658	32.3		40.908 41.228	70.578 70.903	1.00 17.13	6
ATOM	3070	CG2	VAL	658	34.5		42.151	70.055	1.00 15.29	6
ATOM	3071	c	VAL	658	33.5		39.602	72.697	1.00 15.57	6
ATOH	3072	ō	VAL	658	33.0		38.519	72.336	1.00 16.39	8
MOTA	3073	N	ASP	659	33.1		40.225	73.818	1.00 15.80	7
ATOM	3074	CA	ASP	659	32.2	217	39.660	74.762	1.00 16.22	6
ATOM	3075	CB	ASP	659	32.6		39.583	76.152	1.00 18.33	6
ATOM	3076	CG	ASP	659	31.6		39.320	77.262	1.00 17.02	6
ATOM	3077		ASP	659	31.		40.220	78.127	1.00 16.96	9
ATOM ATOM	3078 3079	C	ASP ASP	659 659	31.1 30.9		38.238 40.488	77.248	1.00 15.05	8
ATOM	3080	ò	ASP	659	30.9		41.480	74.877 75.641	1.00 17.09	6 3
ATOM	3081	N	VAL	660	29.		40.096	74.127	1.00 17.40	7
ATOM	3082	CA	VAL	660	28.		40.775	74.150	1.00 18.10	
ATOM	3083	CB	VAL	660	27.1	335	40.550	72.857	1.00 15.37	6
ATOM	3084	CG1		660	28.	760	40.397	71.683	1.00 16.34	ó
ATOM	3085		VAL	660	26.		39.368	72.990	1.00 15.04	5
ATOM	3086	C	VAL	660	27.		40.299	75.335	1.00 20.40	5
ATOM	3087	ō.	UAL	660	27.		39.092	75.635	1.00 21.69	8
ATOM	3088 3089	N	SER	661	27.0		41.218	75.943	1.00 22.33	7
ATOM ATOM	3090	CB	ser Ser	661 661	26.: 27.:		40.865 40.683	77.104 78.308	1.00 23.37	6
ATOM:	3091	OG	SER	661	20.		39.569	78.169	1.00 23.56	6 8
ATOM		·c	SER	661	25.		41.882	77.544	1.00 25.29	6
ATOM:	3093	9	SER	661	24.		42.901	76.839	1.00 24.57	a
MOTA	3094	N	ALA	662	24.	676	41.596	78.784	1.00 26.02	7
ATOM:	3095	CA	ALA	662	23.	690	42.325	79.598	1.00 23.48	ń
ATOM	3096	CB	ALA	662	23.		43.856	79.493	1.00 24.66	5
ATOM	3097	c	ALA	662	22.		41.933	72.339	1.00 22.08	ń
atom atom	3098 3099	М	ALA	662	21.		40.739	79.266	1.00 16.69	3
ATOM	3100	CA	GLY	663 663	21. 19.		42.948	72.300	1.00 23.15	7
ATCM	3101	C	GLY	663	19.		42.775	79.047 80.038	1.00 24.87	5 5
ATOM	3102	ŏ	GLY	663	18.		40.929	79.649	1.00 22.72	3
ATOM	3103	N	ASN	664	19.		42.453	81.277	1.00 24.09	7
ATOM	3104	CA	ASN	654	18.		41.815	82.410	1.00 25.56	÷
ATOM	3105	CF	ASN	664		157	42.706	82.938	1.00 27.33	ń
ATCM:	3106	CG	ASN	664		907	42.725	82.013	1.00 28.05	- 5
ATCN:	3107		ASN	664		791	43.578	81.114	1.00 29.36	3
atom atom	310B 3109	C	NZA S	664 664		939	41.852	82.294	1.00 26.86	٠,
ATOM	3110	٥	ASN	664		831 976	40.352 39.992	82.334 81.488	1.00 25.76	ý a
ATOM	3111	N	GLY	665		250	39.517	83.243	1.00 25.92	8
ATOM	3112	CA	GLY	665		91B	38.123	82.294	1.00 24.29	6

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ATOM	3113	С	GLY	665		8.560	37.239	82.23		00 23.9		
ATOM	3114	ō	GLY	665		8.754	36.011	82.45		00 24.0: 00 22.3:		
MOTA	3115	N	ALA	666		LB.767	37.805 37.054	81.04		00 22.7	-	
MOTA	3116	CA	ALA	666		19.457 19.331	37.724	78.69		00 21.9	_	
ATOM	3117	CB C	ala Ala	666 666		20.893	37.166	80.57		00 24.3		
ATOM ATOM	3118 3119	Ö	ALA	666		21.300	38.225	81.07		00 25.1		
ATOM	3120	N	GLY	667		21.579	36.036	80.67		00 25.5 00 26.4		
MOTA	3121	CA	GLY	667		22.941	36.05B 35.946	81.15 79. 9 4		00 28.1	_	
MOTA	3122	C	GLY	667 667		23.838 24.789	35.145			00 29.4		
ATOM	3123	O N	GLY SER	668		23.483	36.689			00 28.7	3 7	
MOTA MOTA	3124. 3125	CA	SER	668		24.256	36.669	77.64		00 28.0	_	
MOTA	3126	ÇB	SER	668		23.634	37.605			00 28.8		
ATOM	3127	05	SER	668		24.312	37.574 37.209			.00 24.5 .00 27.6		
ATOM	3128	Ç	SER	668 668		25.597 25.647	38.220			.00 27.		
ATOM	3129 3130	O N	SER Val	669		26.623	36.397			.00 26.		7
atom atom	3131	CA	VAL	669		28.049				.00 23.		5
ATOM	3132	СВ	VAL	669		28.665				.00 20.	-	6 5
ATOM	3133		VAL	669		28.460				.00 19.4		6
MOTA	3134		VAL	669		30.175				.00 21.		5
ATOM	3135	C	Val Val	669 669		29.846				.00 20.		E
ATOM	3136 3137	O N	GLN	670		27.845				.00 20.		7
MOTA MOTA	313B	CA	GLN	670		28.193	36.00			.00 18.		6
ATOM	3139	CB	GLN	670		27.005				.00 17.		6 €
ATOM	3140		GLN	670		27.182				.00 22.		6
ATOM	3141	CD	GLN L GLN	670 670		28.500				.00 24.		8
ATOM ATOM	3142 3143		2 GLN	670		27.912		5 69.6	34 1	.00 23.		7
ATOM	3144	-	GLN	670		29.51				.00 17.		6 B
MOTA	3145		GLN	670		29.79				1.00 15. 1.00 15.		7
ATOM	3146		ARG	671		30.33				1.00 16		6
MOTA	3147		ARG	671 671		32.67				1.00 17		6
atom atom	3148 3149			671		32.94				1.00 19		6
ATOM	3150			671		32.49	3 35.26			1.00 18		6
ATOM	3151		ARG	671		32.98				1.00 19 1.00 19		7 6
ATOM	3152			671		33.86				1.00 17		ĭ
ATOM	3153		1 ARG	671 671		34.37 34.30				1.00 17		7
MOTA	3154 315		ARG	671		31.86			158	1.00 18		6
ATOM	315		ARG	671		31.42				1.00 20		8 7
ATOM	315		VAL	672		32.57			460 049	1.00 18		6
ATOM	315			672		32.87 32.07		-	160	1.00 15		5
MOTA	315 316		B VAL 31 VAL	672 673		30.64			682	1.00 17		ř
HOTA MOTA	316		52 VAL	67		32.72		02 68.	133	1.00 17		5
ATOM	_	-	VAL	67:		34.3			849	1.00 14		6
ATOM	_		VAL			34.9			358	1.00 14		8
ATOM						35.01 36.41		_	. 184 . 911	1.00 14		6
ATOM						36.9			150	1.00 1	1.98	5
MOTA MOTA						36.6		25 65.	. 601	1.00 2	1.07	5
ATOM		8 0	D GLU	67	3	36.9			. 759	1.00 2		8
ATOM	310		E1 GL			36.9			.300 .537	1.00 2	3.59	9
ATON			E2 GLI) 67) 67		37.2 36.6			.978	1.00 1	4.79	5
ATOM ATOM						35.6	88 37.4	420 66	. 456	1.00 1	5.66	9
ATO			IL			37.6			.708	1.00 1		7
ATO			A IL	E 6°		38.2			.790	1.00 1		÷
ATO			B IL	_	14	38.3			.498	1.00 1		÷
ATO			G2 IL		74	38.7 37.0			.289	1.00 1	5.11	÷
ATO			CG1 IL	-	74 74	35.6	_		.489	1.00 1	2.07	5 5 5
ATO: ATO			C IL		74	39.	596 37.	922 65	1.198	1.00 1		÷ 3
ATO			o II		74	40.	511 37.		3.909	1.00 1		3
ATO			N LE	r 6	75	39.			3.884	1.00 1		7 5
ATO	M 31	82	CA LE		75	41.	_		3.251 L.744	1.00		á
ATO			CB LE		75 75	40. 40.			1.359	1.00		- 5
ATO ATO			CG LE CD1 LE		75 75	38.			1.326	1.00	13.53	5
ATO			CD2 LE		75	40.	967 35.	743 6	0.014	1.00		5
ATC	M 31	87	c LI	:U 6	75				3.585	1.00		خ :۱
ATC		88	o u		75				3.920 3.521	1.00		,,
ATC		189 190			76 76				3.829			ń
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ATOM	3191	CB	GLU	676	45.667	38.907	63.526	1.00 12.08	
ATOM	3192	CG	GLU	676	45.627		62.478	1.00 11.18	
ATOM	3193	CD	CLU	676	45.494		63.080	1.00 13.77	
ATOM ATOM	3194		GLU	676	46.538		63.546	1.00 16.32	
ATOM	3195 3196	C C	GLU	676	44.367		63.108	1.00 13.00 :	
ATOM	3197	ò	era era	676 676	44.268		63.146	1.00 12.13 #	
ATOM	3198	N	SLY	677	43.569 45.030		62.159	1.00 12.89	
ATOM	3199	CA	GLY	677	45.121		63.699 63.145	1.00 11.52	
ATOM	3200	C	GLY	677	43.796		62.961	1.00 11.07 E	
ATOM	3201	0	SLY	677	43.770		62.523		
ATOM	3202	N	arg	678	42.700		63.329	1.00 14.32 ÷ 1.00 12.98 ÷	
ATOH	3203	CA	ARG	678	41.387		63.174	1.00 14.43 €	
ATOM	3204	CB	ARG	678	40.342		62.927	1.00 13.34 €	
ATOM ATOM	3205 3206	CD	ARG ARG	678	39.529		61.695	1.00 15.05	
ATOM	3207	NE	ARG	678 678	40.401	–	60.504	1.00 17.70 5	
ATOM	3208	cz	ARG	678	41.014 41.887		60.643	1.00 22.61	
ATOM	3209		A.P.G	678	42.274		59.787 58.700	1.00 23.28 €	
ATOM	3210		ARG	678	42.380		60.037	1.00 22.06	
ATOM	3211	С	ARG	678	41.001		64.420	1.00 14.43 €	
ATOM	3212	0	ARG	678	41.199	44.034	63.529	1.00 15.07	
ATOM	3213	N	THR	679	40.462		64.249	1.00 13.15	
ATOM	3214	CA	TEP	679	40.027		65.390	1.00 14.13	
MOTA MOTA	3215 3216	CB OG1	THP.	679	40.996		65.669	1.00 14.19	
ATOM	3217	CG2	THE	679 679	41.204		64.448	1.00 17.57	
ATOM	3218	C	THE	679	42.332 38.637		66.229	1.00 13.59	
ATOM	3219	ō	THR	679	38.393		65.182	1.00 16.43 -	
ATOM	3220	N	GLU	680	37.732		65.540 64.604	1.00 15.23	
ATOM	3221	CA	GLU	680	36.358		64.332	1.00 10.03	
ATOM	3222	CB	GLU	680	36.289		63.128	1.00 19.04 f 1.00 18.69 f	
ATOM	3223	CG	GLU	680	36.140		61.755	1.00 18.32	
ATOM	3224	CD	CTD	680	35.086		60.847	1.00 18.05	
ATOM	3225		GLU	680	34.342	:	60.138	1.00 16.53	
atom Atom	3226 3227	OE2 C	GLU	680	35.019		60.825	1.00 14.40	
ATOM	3228	ò	GLU	680 680	35.489 35.887		64.076	1.00 21.29 4	
ATOM	3229	N	CYS	681	34.299		63.364	1.00 22.54	
ATOM	3230	CA	CYS	681	33.382		64.654 64. 49 8	1.00 22.91 7 1.00 24.61 2	
ATOM	3231	CB	CYS	681	33.617		65.603	1.00 26.42 5	
ATOM	3232	SG	CYS	681	32.134	42.836	66.606	1.00 26.71 15	
ATOM	3233	C	27.5	681	31.958		64.540	1.00 24.30 -	
ATOM ATOM	3234 3235	N	CYS	681	31.579		65.448	1.00 23.84	
ATOM	3236	CA	721	682 682	31.181 29.818	44.688	63.517	1.00 21.58	
ATOM	3237	CB	721	682	29.433		63.511	1.00 20.10	
ATOM	3238	CG1	711	682	30.190		62.131 60.969	1.00 18.07 £ 1.00 16.40 £	
MOTA	3239	CG2	7AL	682	27.952		61.867	1.00 16.40 £ 1.00 17.19 £	
ATOM	3240	C	7AL	682	28.961	44.077	64.001	1.00 17.00	
ATOM	3241	0	VAL	682	28.659	43.049	63.342	1.00 15.10	
ATOM	3242	N	LEU	683	28.449		65.258	1.00 17.47	
ATOM	3243	CA	LEU	683	27.485	43.294	65.859	1.00 20.70 -	
ATOM ATOM	3244 3245	CB	120	683	27.326		67.348	1.00 17.50 :	
ATOM	3246	CD1	LEC	683 683	28.420 28.201		68.299	1.00 13.82	
ATOM	3247	CD2		683	28.201		69.667 68.387	1.00 13.45 -	
ATOM	3248			683	26.228		65.104	1.00 15.36 £ 1.00 24.03 £	
ATOM	3249	0	120 120	683	25.446		65.544		
ATOM	3250	N	SĒR	684	26.087		63.914	1.00 24.27 = 1.00 25.99	
ATOM	3251	CA	SEP.	684	25.003		63.028	1.00 26.98	
ATOM	3252	CB	SEP.	684	25.222		61.629	1.00 31.20	
ATOM ATOM	3253	OC	327.	684	26.502		61.067	1.00 36.99	
ATOM	3254	Ç	JER.	684	23.614		63.491	1.00 26.69	
ATOM	3255 3256	Ó N	eer Aen	584 685	22.800 23.397		63.699	1.00 27.76	
ATOM	3257	ÇA	ASS	685	22.049		63.826	1.00 24.94	
ATOM	3258	CB	AII	685	21.716		64.131 63.083	1.00 25.85	
ATOM	3259	CG	ASN	685	22.993		62.504	1.00 27.66 : 1.00 28.61 :	
ATOM	3260		AJ:	685	23.994		62.186	1.00 28.61	
ATOH	3261	ND2	ZEA	685	22.972	38.406	62.407	1.00 28.57	
ATOM	3262	C	ASN.	685	21.748	40.978	65.533	1.00 26.76	
ATOM	3263	÷.	A.:::	685	22.271		€5.923	1.00 27.14	
hota Mota	3264 3265	N	111	686	20.899		66.287	1.00 27.14 ± 1.00 25.95	
ATOM	3266	CA CB		686 686	20.583		67.649	1.00 24.26	
ATOM	3267	CG	LEU	686	21.779 22.718		68.584 68.474	1.00 22.44 5	
ATOM	3268		12:	686	23.700		69.708	1.00 23.47 E	
								64.04	

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ATOM	3269	CD2		686		563	42.742	67.17 68.37	-	00 20.4 00 26.4		
ATOM	3270	C	LEU	686 686		233 361	41.566	68.4		00 27.	06 8	ı
ATOM ATOM	3271 3272	O N	LEU ARG	687		035	42.801	68.8	58 1.	00 25.		
ATOM	3273	CA	ARG	687	17.	838	43.147			00 21.	-	5
ATOM	3274	CB	ARG	687		117	42.901	71.1		00 21. 00 18.		5
MOTA	3275	CG	ARG	687		. 254 . 778	41.847			00 20.		ś
ATOH	3276	CD	ARG ARG	687 687		. 883	39.426		-	00 23.	57	7
MOTA	3277 3278	NE CZ	ARG	687		832	38.188		16 1.	00 24.		÷
MOTA	3279		ARG	687		. 636	37.837			00 25.		7
ATOM	3280		ARG	687		. 969	37.303			.00 23.		7 5
ATOM	3281	С	ARG	687		. 358	44.587		_	.00 23. .00 24.		3
ATOM	3282	0	ARG	687		.863 .420	45.369			.00 23.		7
ATOM	3283	N	GLY GLY	688 688		.825	46.263			.00 22.		5
atom Atom	3284 3285	CA	GLY	688		.583	46.644	71.8		.00 23.		6
ATOM	3286	ŏ	GLY	688	15	.359	45.760			.00 21.		8
ATOM	3287	N	ARG	689		.712	47.94			.00 23.		7
MOTA	3288	CA	ARG	689		.531	48.53			.00 23.		6
ATOM	3289	CB	ARG	689		.034	48.51			.00 20		6
ATOM	3290	CG	ARG	689 689		.543	50.98			.00 1B		6
ATOM	3291	CD	arg arg	689 689		.071	52.26			.00 17		7
ATOM	3292	NE CZ	ARG	689		.201	52.82			.00 19	. 24	5
MOTA MOTA	3293 3294		ARG	689		.738	52.25	3 76.2		.00 12		7
MOTA	3295		ARG	689	14	1.704	54.06			.00 18		7
ATOM	3296	С	ARG	689		5.425	47.95			.00 25		B
ATOM	3297	0	ARG	689		5.512	48.54			.00 25		7
MOTA	3298	N	THR	690		7.153 B. 05 3	46.88 46.12			.00 23		6
MOTA	3299	CA	THR THR	690 690		B.530	44.90			.00 24		6
ATOM ATOM	3300 3301		1 THP.	690		7.550			405	1.00 24	.96	8
MOTA	3302		2 THR	690		8.808				1.00 24		5
ATOM	3303	-	THR	690		9.337				1.00 27		6
ATOM	3304		THR	690		0.052				1.00 2		8 7
ATOM	3305	N	ARG	691		9.653				1.00 20 1.00 21		6
MOTA	3306			691		0.920				1.00 2		6
ATCH	3307			691		0.908 1.668				1.00 3		5
ATOM	3308			691 691		1.736				1.00 3		5
MOTA MOTA	3309 3310			691		2.360	45.5	49 82.		1.00 2		7
ATOM	3311			691	2	1.6B1				1.00 3		5
ATOM	3312	NI S	11 ARG	691		20.331	44.6			1.00 3 1.00 2		7
MOTA	3313	_	12 ARG	691		22.33			.768 .114	1.00 2		ń
ATOM	331		ARG	691		22.024 21.86			. 231	1.00 2		8
ATOM	331		ARG Tyr	691 692		23.15			. 682	1.00 2		7
MOTA MOTA	331			692		24.21			. 256	1.00 2	3.54	5
ATOM	331			692		24.23	7 45.8		.744	1.00 2		á
ATON	331			692		23.31			.100	1.00 2		ó S
ATOM	332	0 C	D1 TYR			23.30			.501	1.00 2		6
ATOM	332		E1 TYR			22.54 22.53			.833	1.00 2		5
ATOM	332		D2 TYR E2 T YR			22.33 21.75		-	. 325	1.00 2		6
ATOM			Z TYP			21.77			.745	1.00 2		5
ATOM ATOM			H TYP			21.02	1 42.0	086 72	.059	1.00		8
ATOM						25.53	4 46.		5.739	1.00		6
ATOM		?7 C				25.77			5.606 7. 30 2	1.00		8
ATOM						26.38			7.758	1.00		6
ATOM			A THI			27.87			9.301	1.00		5
ATOR			OG THI			26.74			9.909	1.00		Я
ATO:			CG2 TH			29.1			9.685	1.00	12.28	ń
ATO:			C TH			28.7	03 45.	-	7.062		14.45	÷
ATO			O TH	R .693		28.4			6.926		11.01	8 7
ATO	4 33	35	N PH			29.8			6.604 5.845		15.34 15.68	6
ATO			CA PH			30.8	_		4.405		18.12	6
ATO			CB PH CG PH			29.4			3.816		19.49	6
ATO ATO			CD1 PH			28.7			4.043	1.00	18.66	6
ATO			CD2 PH			28.8	82 44		3.015		18.42	
ATO			CE1 PH	E 694		27.4		_	3.481		19.71	
ATO		42	CE2 PH			27.6			72.450		16.44	
ATO		43	CZ PE			26.9			72.679 76.374		14.83	
ATC		144	C Pi			32.2			76.835		14.75	3
ATC		145 146	N Al			33.1			76.155		14.22	

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ATOM	3347	CA	ALA	695	34.532	44.271	76.533	1.00 14.58 6
MOTA	3348	CB	ALA	695	34.704	43.821	77.959	1.00 15.52 6
ATOM	3349	С	ALA	695	35.331	43.352	75.579	1.00 16.59 6
ATOM	3350	0	ALA	695	34.739	42.503	74.883	1.00 16.77 6
ATOM	3351	N	VAL	696	36.663	43.475	75.554	1.00 18.89 7
atom Atom	3352 3353	CA CB	VAL VAL	696 696	37.475	42.637	74.640	1.00 18.54 6
ATOM	3354	CG1	VAL	696	37.455 37.867	43.242 44.705	73.198	1.00 19.19 6
ATOM	3355	CG2		696	38.335	42.446	73.223 72.255	1.00 17.15 6 1.00 20.60 6
MOTA	3356	С	VAL	696	38.923	42.284	75.047	1.00 18.64 6
ATOM	3357	0	VAL	696	39.654	43.093	75.637	1.00 18.43 8
ATOM	3358	N	ARG	697	39.321	41.055	74.738	1.00 18.97 7
atom atom	3359 3360	CA CB	ARG ARG	697 697	40.675	40.563	75.050	1.00 18.67 6
ATOM	3361	CG	ARG	697	40.593 39.772	39.173 39.078	75.664 76.889	1.00 17.03 6
ATOM	3362	CD	ARG	697	39.842	37.650	77.417	1.00 15.40 6 1.00 18.07 6
ATOM	3363	NE	ARG	697	39.077	36.676	76.632	1.00 18.07 6 1.00 17.47 7
ATOM	3364	CZ	ARG	697	38.722	35.467	77.081	1.00 19.24 6
ATOM	3365	NH1	ARG	697	39.061	35.078	78.309	1.00 20.70 7
ATOM	3366		ARG	697	38.014	34.643	76.318	1.00 18.93 7
atom atom	3367 3368	0	ARG ARG	697	41.625	40.494	73.818	1.00 18.98 6
ATOM	3369	N	ALA	697 698	41.180 42.926	40.255 40.660	72.677	1.00 19.20 8
ATOM	3370	CA	ALA	698	43.973	40.609	74.077 73.057	1.00 17.10 7 1.00 14.99 6
ATOM	3371	CB	ALA	698	44.816	41.858	73.146	1.00 14.99 6 1.00 15.98 6
ATOM	3372	С	ALA	698	44.838	39.366	73.296	1.00 14.49 6
ATOM	3373	0	ALA	698	45.073	38.999	74.432	1.00 16.90 8
ATOM	3374	N	ARG	699	45.349	38.753	72.234	1.00 13.57 7
ATOM	3375	CA	ARG	699	46.174	37.540	72.325	1.00 10.72 6
ATOM ATOM	3376 3377	CB CG	ARG ARG	699 699	45.229	36.331	72.392	1.00 12.04 6
ATOM	3378	CD	ARG	699	45.692 46.738	35.014 34.349	71.794	1.00 12.63 6 1.00 20.39 6
ATOM	3379	NE	ARG	699	46.913	32.910	72.399	1.00 20.39 6 1.00 21.37 7
YLON	3380	CZ	ARG	699	46.119	31.955	72.895	1.00 21.92 6
ATOM	3381	NH1	ARG	699	45.069	32.257	73.672	1.00 21.47 7
MOTA	3382	NH2		699	46.442	30.682	72.710	1.00 22.33 7
MOTA MOTA	3383 3384	0	ARG	699	47.090	37.470	71.094	1.00 9.38 6
ATOM	3385	N	arg Met	699 700	46.680 48.355	37.820 37.109	69.991	1.00 10.86 8
ATOM	3386	CA	MET	700	49.263	37.029	71.282 70.140	1.00 8.21 7 1.00 7.21 6
ATOM	3387	CB	MET	700	50.724	36.955	70.551	1.00 7.21 6 1.00 6.01 6
ATOM	3388	CG	MET	700	51.322	38.292	70.963	1.00 5.33 6
ATOM	3389	SD	MET	700	52.092	39.250	69.678	1.00 9.84 16
MOTA	3390	CE	MET	700	51.368	40.792	69.955	1.00 8.49 6
atom atom	3391 3392	0	met Met	700 700	48.875	35.808	69.375	1.00 6.64 6
ATOM	2393	Ŋ	ALA	701	48.609 48.849	34.755 35.943	69.939	1.00 6.32 8 1.00 7.50 7
ATOM	3394	CA	ALA	701	48.425	34.837	67.250	1.00 7.50 7 1.00 8.94 6
ATOM	3395	CB	ALA	701	47.605	35.361	66.065	1.00 7.41 6
ATOM	3396	C	ALA	701	49.483	33.855	66.779	1.00 9.12 6
ATOM	3397	0	ALA	701	50.679	34.165	66.639	1.00 9.86 3
MOTA	3398	N CA	GLU GLU	702	48.980	32.669	66.491	1.00 10.01 7
ATOM	3399 3400	CB	GLU	702 702	49.763 48.971	31.574 30.275	65.987	1.00 13.16 6
ATOM	3401	CG	GLU	702	48.724	29.784	66.108 67.501	1.00 15.92 6
ATOM	3402	CD	GLU	702	48.597	28.284	67.507	1.00 18.17 6 1.00 21.01 5
MOTA	3403	OE1	GLU	702	47.904	27.731	66.611	1.00 22.10 8
MOTA		. OE 2		702	49.233	27.652	68.377	1.00 24.81 8
ATOM	3405	C	GLU	702	50.126	31.770	64.510	1.00 13.07 6
atom Atom	3406 3407	0 N	GLU PRO	702 703	49.560	32.617	63.802	1.00 12.10 8
ATOM	3408	CD	PRC	703	51.106 51.501	30.986 30.820	64.037 62.625	1.00 14.95 7
ATOM	3409	CA	PRC	703	51.783	30.007	64.899	1.00 17.31 6 1.00 14.84 6
ATOM	3410	CB	PRC.	703	51.896	28.794	63.999	1.00 14.77 6
ATOM	3411	CG	PRC	703	52.253	29.467	62.635	1.00 19.35 6
ATOM	3412	С	PRO	703	53.150	30.488	65.409	1.00 13.50 5
ATOM	3413	0	PRC	703	53.801	29.774	66.157	1.00 15.09 B
ATOM ATOM	3414 3415	n Ca	SER	704	53.587	31.681	65.002	1.00 11.82 7
ATOM	3415	CR	ser ser	704 704	54.873 55.156	32.218 33.574	65.461 64.798	1.00 9.78 5
ATOM	3417	36	SER	704	55.301	33.574	63.394	1.00 9.23 6 1.00 8.65 H
ATOM	3418	С	SER	704	54.860	32.386	67.003	1.00 B.65 B 1.00 11.09 5
ATOM	3419	9	5ER	704	55.621	31.729	67.736	1.00 12.01 a
ATOM	3420	N	PHE	705	53.937	33.229	67.468	1.00 8.75 7
ATOM ATOM	3421 3422	CA CB	PHE PHE	705	53.767	33.532	68.857	1.00 3.52 6
ATOM	3423	CG	PHE	705 701	53.323 54.159	34.973 35.924	68.988 68.184	1.00 5.09 6
ATOM	3424		PHE	705	53.696	35.924	68.184 66.957	1.00 7.49 6
				-	23.000			1.00 8.92 6

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ATOM	3425	CD2	PHE	705		55.4		36.2		8.611	1.00	8.54	:
ATOM	3426	CE1	PHE	705		54.5	-	37.2		66.163 67.833	1.00	7.44	÷
MOTA	3427		PHE	705 705		56.2 55.8		37.1 37.5		66.606	1.00	5.19	ŧ
MOTA	3428 3429	CZ C	PHE PHE	705		52.7		32.5	91 (69.505	1.00	5.11	5
atom atom	3430	ò	PHE	705		52.2		31.6		68.878	1.00	4.57	3 7
ATOM	3431	N	GLY	706		52.6		32.7		70.809	1.00	8.69 7.99	ė
ATOM	3432	CA	GLY	706		51.7		31.5		71.622 72.932	1.00	9.39	:
MOTA	3433	Ç	GLY	706 706		51.6		33.		73.069	1.00	9.05	;
MOTA	3434 3435	0 N	GLY	707		50.8		32.2		73.878		10.91	7
ATOM	3436	CA	GLY	707		50.		32.		75.162	1.00	9.87	÷
ATOM	3437	С	GLY	707		49.		32.		75.977 76.063	1.00	7.80	÷
MOTA	3438	0	GLY	707 708		48.		31.°		76.540	1.00	7.59	_
ATOM	3439 3440	N CA	PHE	708		47.		33.		77.372	1.00	B.42	
atom atom	3441	CB	PHE	708		48.		33.		78.874	1.00	9.14	
ATOM	3442	CG	PHE	708		49.		33.		79.277	1.00	8.19 5.98	
ATOM	3443		PHE	708 708			196 638	31.	679	79.352	1.00	6.32	
ATOM	3444 3445		PHE PHE	708			296		016	79.974	1.00	8.74	5
MOTA MOTA	3446		PHE			51.	730		912	79.731	1.00	5.05	
ATOM	3447	CZ	PHE	708			570		587	80.040	1.00	4.00 7.99	
ATOM	3448	C	PHE				846 260		066 187	77.077 76.721	1.00	6.94	
MOTA	3449	0	PHE TPP				562		777	77.285	1.00	9.0	9 7
atom Atom	3450 3451	N CA	TRP				475		752	77.119		12.1	
ATOM	3452		TRP)		114		.083	77.396	-	11.5	_
MOTA	3453		TRE				417		. 592 . 354	76.165 74.999	1.00	12.0	
ATOM	3454		2 TRI 2 TRI				. 098 . 465		.481	74.092	1.00		2 ÷
ATOM ATOM	3455 3456		3 TRI				. 283		. 687	74.634	1.00		9 -
ATOM	3457	_	1 TRI				. 971		.326	75.929		11.5	
ATOM	3458	NE	1 TR				. 398		.250	74.688	1.00	12.1	
ATOM	3459		2 TR				.018 . 83 6		.897 .103	73.399		11.5	_
MOTA	3460 3461		3 TRI 12 TRI				.214		.209	72.513		10.5	4 5
atom Atom	3462		TR				. 635		. 973	78.056		10.5	
ATOM	346		TR				.770		. 823	79.268		0 12.1 0 11.5	
MOTA	346		SE				. 620 . 765		.177	77.508		0 12.1	-
MOTA MOTA	346: 346:		_				.040		.594	77.50			78 ∻
ATOM	346						. 847		. 258	77.15		0 10.0	
ATOM	346		SE				. 522		9.567 9.832	79.21 79.13		0 12.2 0 17.2	
MOTA	346						2.531 3.580).563			0 12.	01 7
ATOM ATOM	347 347						2.43		.867	80.89		0 12.	49 -
ATOM		-		_			2.85	-	1.817			0 12.	
ATOM	347						1.43		1.560 2.073			0 13. 0 14.	
ATOM					11 12		1.81 0.15		1.558			0 13.	_
ATOM ATOM					12		9.15		2.251			0 12.	
ATOM		-		_	12		7.75		2.031				73 -
ATOM					12		7.20		0.647				57 ÷
ATOM			D2 T		12 12		6.79		8.74				30 ÷
MOTA MOTA			E3 T		12		6.71	8 4	0.60	77.27			.78 ÷
ATON		82 ' (CD1 T	rp 7	12		7.03		9.64				.29
ATON			NE1 T		12		6.57 5.96		8.49				46
ATO: ATO:			CZ2 T C23 T		12 12		6.27		39.77			90 7.	.52 -
ATO			CH2 T		112		15.90		8.43				.00 :
ATO					112		39.49		13.74			00 12 00 12	ה צכ. ב חו
ATO					112		40.12 39.1		14.26 44.38		95 I.	20 15	.32
ATO: ATO:					713 713		39.3		45.81		66 i.	30 15	.45
ATO					713		39.2	94	46.10	8 75.6	59	00 14	.50
ATO	M 34	92	OG S	SEP	713		37.9		45.89			30 11 00 15	
ATO		93			713		38.1 37.0		46.48 45.90			00 18	. 64
ATO ATO		194 195			713 714		38.3		47.70		79 1.	.00 17	.04
ATO		196			714		37.1	63	48.39	91 79.8	88 1.	.00 20	.29
ATO	M 34	197	СВ	GLU	714		37.5		49.80		76 _	. 50 21 . 80 24	.54 .61
ATO		198		GLU	714		38.4		49.83		78	.00 24 .00 24	5.47
ATC ATC		499 500	OE1 CD	GLU GLU	714 714		39.8		51.4			.00 2	
ATC		501	OE2		714		37.7	35	52.0	74 81.5		.00 2	
ATC		502	С	GLU	714		35.6	885	48.3	66 79.0	127 :	.00 2	1.46

bref2	lc.p	i b		Thu	Apr 25	12:27:47	1996	46	
ATOM	3503	0	GLU	714	35.86	7 48.844	77.886	1.00 21.24	а
ATOM	3504	N	PRO	715	34.78		79.611	1.00 20.46	7
ATOM	3505	CD	PRO	715	34.70		81.090	1.00 21.13	5
ATOM	3506	CA	PRO	715	33.46	0 47.694	79.015	1.00 19.23	5
ATOM	3507	CB	PRO	715	32.62	7 47.183	80.182	1.00 21.32	6
ATOM	3508	CG	PRO	715	33.22		81.352	1.00 19.98	5
ATOM	3509	С	PRO	715	32.87		78.473	1.00 20.02	5
ATOM	3510	0	PRO	715	33.19		78.922	1.00 20.10	à
ATOM	3511	N	VAL	716	31.93		77.562	1.00 20.51	7
MOTA	3512	CA	VAL	716	31.22		76.910	1.00 19.79	5
ATOM	3513	CB	VAL	716	31.76		75.440	1.00 18.56	5
ATOM	3514	CG1		716	30.98		74.396	1.00 18.80	5
ATOM	3515		VAL	716	31.74		75.099	1.00 16.95	ó
MOTA	3516	C	VAL	716	29.77		76.90B	1.00 21.79	5
ATOM	3517	0	VAL	716	29.51		76.624	1.00 20.72	9
MOTA	3518	N	SER	717	28.85		77.264	1.00 22.27	7
ATOM	3519	CA	SER	717	27.43		77.331	1.00 21.09	5
ATOM	3520	CB	SER	717	26.92		78.764	1.00 23.89	6
ATOM	3521	oc	SER	717	27.18		79.607	1.00 24.17	8
atom Atom	3522 3523	0	SER SER	717 717	26.55		76.375	1.00 20.65	6
ATOM	3524	N	LEU	717	26.54 25.83		76.394	1.00 19.78	а
ATOM	3525	CA	LEU	718	24.86		75.523	1.00 21.29	7
ATOM	3526	CB	LEU	718	25.00		74.585 73.188	1.00 21.71	5
ATOM	3527	CG	LEU	718	24.50		72.057	1.00 17.72 1.00 15.29	5
ATOM	3528		LEU	718	25.27		72.069	1.00 11.08	5
ATOM	3529		LEU	718	24.63		70.733	1.00 11.73	6 5
ATOM	3530	c	LEU	718	23.47		75.183	1.00 22.58	5
ATOM	3531	ō	LEU	718	23.39		76.191	1.00 24.55	3
ATOM	3532	N	LEU	719	22.39		74.564	1.00 23.55	ว
YLOH	3533	. CY	LEU	719.	21.02		75.054	1.00 23.37	5
MOTA	3534	CB	LEU	719	20.63		76.069	1.00 23.00	6
ATOM	3535	CG	LEU	719	21.54	0 51.746	77.325	1.00 22.19	5
ATOM	3536	CD1	LEU	719	21.29	0 53.039	78.084	1.00 19.79	5
ATOM	3537		LEU	719	21.41	6 50.545	78.254	1.00 20.88	6
ATOM	3538	С	LEU	719	19.98	6 50.393	73.904	1.00 23.18	6
ATOM	3539	0	LEU	719	18.88		74.036	1.00 24.17	8
ATOM	3540	N	THR	720	20.32		72.828	1.00 22.42	7
ATOM	3541	CA	THP.	720	19.49		71.597	1.00 21.89	6
ATOM	3542	CB	THP.	720	19.03		71.295	1.00 22.47	6
ATOM	3543	0G1		720	18.79		72.513	1.00 24.25	8
ATOH	3544	CG2		720	20.04		70.444	1.00 20.74	5
MOTA	3545	С	THP.	720	18.26		71.492	1.00 22.94	5
MOTA	3546	0	THP	720	17.14	0 49.947	71.240	1.00 22.69	ā

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Data Set	Resolution	Reflections	Completeness	, Eys	Sites Riso	R _{iso} t	R _{Cullis}	RKraut	Phasing Power	Ower	
400	(Å) 25.0-2.8	(*) 14158	0.93(0.91)	0.05	ı	ı	ı	•			
HgAc ₂	25.0-3.0	11496	0.93 (0.91)	0.10	7	0.102	0.56	0.114	IBO 1.87 (3.1Å) Ano 1.35 (4.0Å)	(3.1Å) (4.0Å)	
UO ₂ (NO ₃) 2	25.0-3.0	11931	0.96 (0.94)	0.14	4	0.116	0.62	0.137	180 1.95 (3.1Å) Ano 1.72 (3.9Å)	(3.1Å) (3.9Å)	
										.12.	
Refinement	Refinement Statistics:			RMS 1	rom ide	RMS from ideal values	88	Average	Average B Value (A-)	(A-)	
Resolution	Resolution Relflections	Total Number of atoms	R-value	Bond Length	ingth	Bond Angle	Ingle	EBP1	EBP2	Peptides	1
								1			
8.0-2.8	13894	3462	0.21		0.01	0.016(Å) 2.1°	2.1	10.5	12.3	10.7	1

*Rsym=[1-<1 / /21.

TRISO El FPH-FP / LFp.

*Roulis El Forte Freeles / For Fp for all centric reflections.

SPhase Power=(El FpH(calc) 2/El FpH(obs) * Fp(calc) | FpH(obs) * Fp(calc) is the lack of closure error to maximum resolution indicated. TRKraut = [] FpH(obs) - FpH(calc) + FpH(calc) - FpH(calc) + FpH(obs) + FpH(obs) for all acentric relfections (anamalous case).

^aCompleteness of data in the outer shall, $(2.9-2.8\mbox{\AA})$ for the native and $(3.1-3.0\mbox{Å})$ for both derivatives. Hean Figure of Merit=< $P(\alpha)e^{i\alpha}/LP(\alpha)l>$ where $P(\alpha)$ is the phase probability.

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Peptidel-EBP1	Peptidel-EBP2	Peptidel-EBP2	Peptide2-EBP1	Peptide2-EBP1 Peptide1-Peptide2
Gly ^{P9} O-Het ¹⁵⁰ N	Tyr ^{P4} OH-Ser ⁹² N	Gly ^{P9} O-Met ¹⁵⁰ N	Tyr ^{p4} OH-Ser ⁹² N Tyr ^{p4} O-Cys ^{p6} N	Tye ^{p4} o-cyb ^{p6} n
Pro ^{P10} 0-Thr ¹⁵¹ N		Pro ^{P10} 0-Thr ¹⁵¹ N		Tyr ^{p4} N-Cyg ^{p6} O
Pro ^{P10} 0-Thr ¹⁵¹ 07		Pro ^{P10} 0-Thr ¹⁵¹ 0 ₇ 1		Cys ^{P6} O-Tyr ^{P4} N
LeuP110-Ser152N		Leu ^{P11} 0-Ser ¹⁵² N		Cys ^{P6} N−1yr ^{P4} O
LeuP110-Ser15207		Leu ^{p11} 0-Ser ¹⁵² 07		

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CLAIMS

What is claimed is:

- 1. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
 - (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- 15 (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.

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- 2. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is cocrystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said criteria data set;
 - (c) outputting to said output device the constructed model.
- 3. A compound having a chemical structure selected using the method of claim 1, said compound being an EPO mimetic.
 - 4. The compound of claim 3 wherein said compound is not a peptide.
 - 5. The compound of claim 3 wherein said compound is a peptide.
 - 6. The compound of claims 5 wherein said peptide has 15 of fewer amino acids.

WO 97/41526

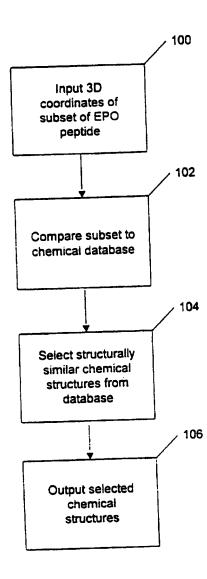


FIG. 1

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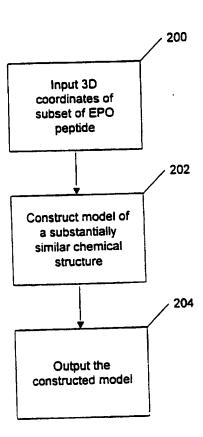


FIG. 2

INTERNATIONAL SEARCH REPORT

International application No. PCT/US97/07218

A. CLAS	SIFICATION OF SUBJECT MATTER		•
IPC(6) :0	G06F 159:00		
US CL :: According to	164/496 International Patent Classification (IPC) or to both nat	tional classification and IPC	
	DS SEARCHED		
Minimum do	cumentation searched (classification system followed b	y classification symbols)	
U.S. : 3	64/496, 497,498,578		
	on searched other than minimum documentation to the e	reet that such documents are include	d in the fields searched
Documentati	on searched other than minimum documentation to the e	ALLIA WIEL GOOD GOOD!	
Electronic da	ata base consulted during the international search (nam	e of data base and, where practicabl	e, search terms used)
ans, dialo			
C. DOC	UMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where app	ropriate, of the relevant passages	Relevant to claim No.
x	US, 5,331,573 A (BALAJI et al.) 19 46-66, col. 13, lines 20-55, col. 14	July 1994, (col. 7, lines 1, lines 12-23	1-6
A,P	US 5,557,535 A (SRINIVASAN et a labstract, fig. 1, col. 4, line 57 - co	al.) 17 September 1996 ol. 6,line 55)	, 1,2
A,P	US 5,555,366 A (TEIG et al.) 10 Se fig. 8, fig. 12)	ptember 1996, (abstract	, 1,2
A	US 5,265,030 A (SKOLNICK et al.) 2, line 20 - col. 3, line 20)	23 November 1993, (col	. 1,2
A,P	MCCARTHY, "Small Peptide De Erythropoietin" Lancet, 8/96 vol. 3	signed that can Mimi 348, no. 24, p.395	1-6
X Furt	her documents are listed in the continuation of Box C.	See patent family annex	
	pocial categories of cited documents: ocument defining the general state of the art which is not considered	"I" later document published after the date and not in conflict with the ap principle or theory underlying the	international filing date or priority plication but cited to understand the invention
<u> </u>	to be part of particular relevance artier document published on or after the international filing date	"X" document of particular relevance	; the claimed invention cannot be sidered to involve an inventive step
0	ocument which may throw doubts on priority claim(s) or which is ited to establish the publication date of another citation or other pecial reason (as specified)		tive step when the document is
.0.	ocument referring to an oral disclosure, use, exhibition or other	combined with one or more other being obvious to a person skilled	such documents, such communications in the art
.b. q	ocument published prior to the international filing date but later than ne priority date claimed	'&' document member of the same p	
	e actual completion of the international search	Date of mailing of the international	search report
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Commirs Box PCT	mailing address of the ISA/US oner of Patents and Trademarks on, D.C. 20231	Authorized officer MELANIE KEMPER	
Facsimile		Telephone No. (703) 305-3900	

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US97/07218

		CT/US97/072	10
C (Continua	tion). DOCUMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where appropriate, of the relevant	passages	Relevant to claim N
	LIVNAH ET AL., "Functional Mimicry of a Protein Hor a Peptide Agonist" Science 26 July 1996, vol. 273 no. 27464-471.	mone by 4, p.	1-6